QD
41
A3312
1976
UNIT
H
C. 3
CURR

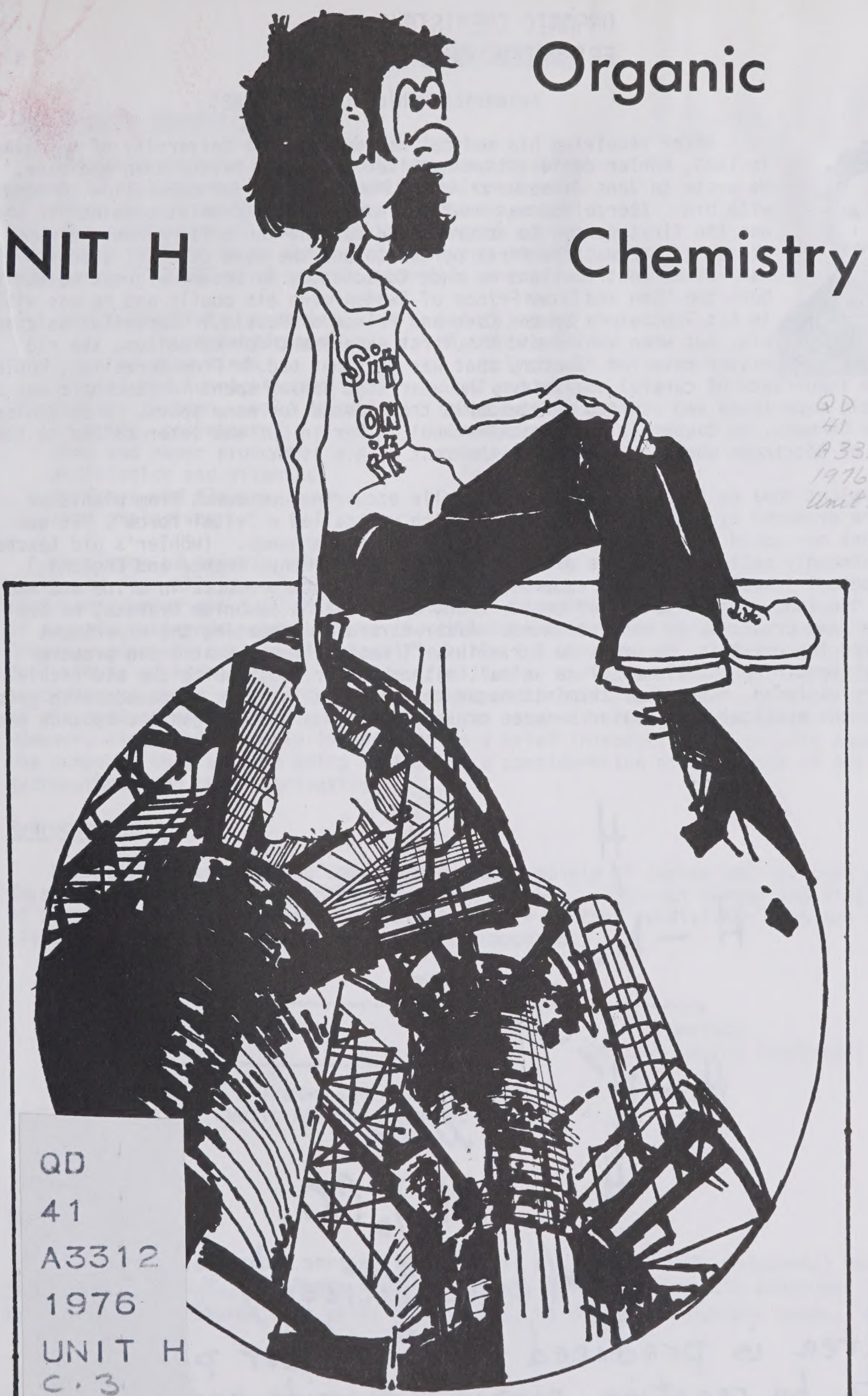
Ex libris
universitatis
albertaensis

Digitized by the Internet Archive
in 2021 with funding from
University of Alberta Libraries

https://archive.org/details/alchem20unithjenk

UNIT H

Organic Chemistry

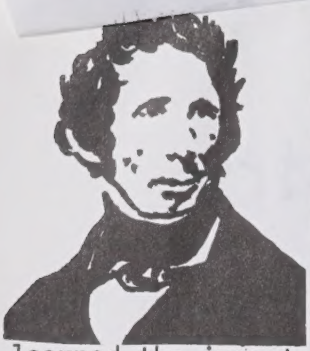


QD
41
A3312
1976
Unit H

QD
41
A3312
1976
UNIT H
C.3

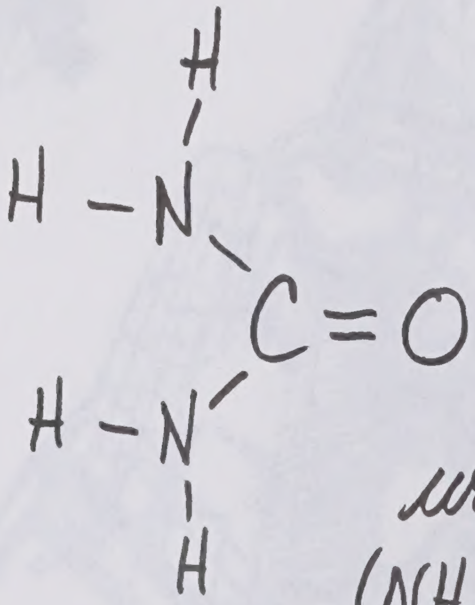
ANIC CHEMISTRY
EDRICH WOHLER

Friedrich Wöhler (1800 - 1882)



After receiving his medical degree from the University of Heidelberg in 1823, Wöhler decided that he liked chemistry better than medicine. He wrote to Jons Jakob Berzelius in Sweden asking for permission to study with him. (Berzelius was another famous doctor-chemist combination who was the first person to accurately determine the molar masses of many elements. He was the first person to use the term catalyst and with the many other contributions he made to science, he became a great celebrity. Both the King and Crown Prince of Sweden were his pupils and he was visited in his laboratory by the Czar and Prince of Russia.) Berzelius welcomed him, but when Wöhler did his first experiment for Berzelius, the old master retorted "Doctor, that was fast but bad." From Berzelius, Wöhler learned the importance of careful analysis. The year that Wöhler spent in Stockholm was a most valuable experience and started a friendship that lasted for many years. When Wöhler returned to Germany, he taught at a technical school in Berlin but was later called to the University of Göttingen where he stayed for the rest of his life.

A prevalent idea at the time was that naturally occurring compounds from plants or animals were produced by some mysterious force which was called a "vital force". It was believed that man would never be able to synthesize these compounds. (Wöhler's old teacher Berzelius strongly believed this, as did most chemists in Germany, France and England.) While in medical school, Wöhler had experimented with the waste products in urine and had often seen the long, thin crystals of urea. When, upon beating ammonium cyanate, he produced these same crystals, he was astounded. After carefully repeating the experiment and analyzing the crystals, he wrote to Berzelius, "I must tell you that I can prepare urea without requiring the kidney of an animal, either man or dog." With the old vital-force theory exploded, many other chemists began to synthesize organic compounds with great success and the mystical distinction between organic compounds and inorganic compounds was eliminated.



urea

$(NH_2)_2CO$

(a fertilizer)

Note: Urea is produced at fertilizer plants in Alberta by reacting carbon dioxide and ammonia.

LIBRARY
UNIVERSITY OF ALBERTA

What Organic Chemistry Is

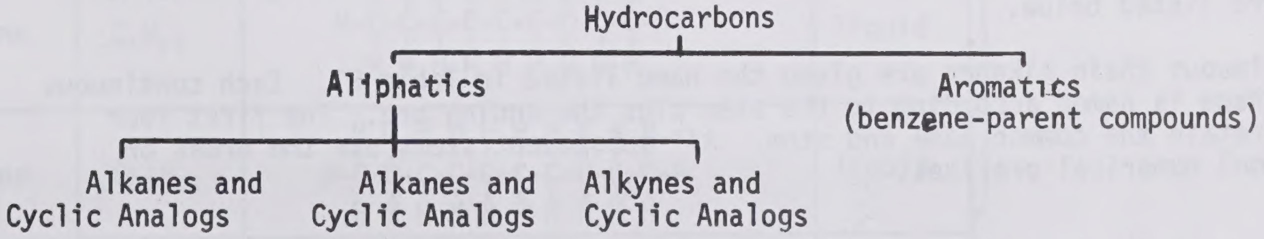
The terms *organic* and *inorganic* are used to distinguish between two different groups of substances. Organic substances are considered to include all compounds of carbon except oxides of carbon, carbonates, carbides and cyanides. These exceptions plus the substances of the remaining elements are considered to be inorganic. Organic substances include those derived from living organisms as well as numerous synthetic substances. Examples of organic materials are:

foodstuffs (fats, proteins, carbohydrates)
fuels of many kinds
greases and lubricating oils
fabrics (cotton, wool, rayon, nylon, polyesters)
wood and paper products
antibiotics and vitamins
perfumes and flavors
some explosives
paints, varnishes and lacquers
plastics and elastomer (e.g. polystyrene and rubbers)
dyes and pigments
soaps and detergents
cosmetics
some agricultural chemicals (some fertilizers, insecticides and pesticides)

Knowledge of organic substances has grown to the extent that presently between three and four million organic compounds are known. By contrast, known inorganic compounds number about 50 000. To establish coherence among the vast array of organic compounds, chemists use the technique of simplification by classification. Organic compounds are usually classified into two main groups - hydrocarbons and derivatives of hydrocarbons. Smaller families or series of compounds are established according to their representative structure and properties. Such a general scheme of classification is used in approaching the study of organic compounds in this unit. However, since this is only intended to be a brief introduction to organic chemistry, the scope in this unit is being limited to a consideration of only some of the simpler hydrocarbons and their derivatives.

Hydrocarbons

Hydrocarbons are organic compounds composed solely of carbon and hydrogen atoms. The atoms are bonded to each other by covalent bonds. The vast number and wide range of complexity of hydrocarbons necessitates their further subdivision into two general classes - aliphatic compounds and aromatic compounds.


Hydrocarbons
Aliphatics
Aromatics
(benzene-parent compounds)
Alkanes and Cyclic Analogs
Alkanes and Cyclic Analogs
Alkynes and Cyclic Analogs

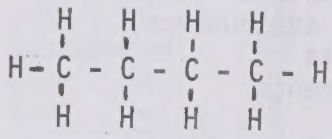
ALKANES

Bonding in Alkanes

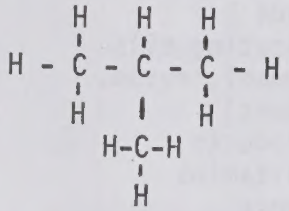
The alkane hydrocarbon series (the simplest class of organic compounds) has the general formula C_nH_{2n+2}. These hydrocarbons are like other organic compounds in that each carbon atom shares four pairs of electrons to form four covalent bonds. All members of this series are called saturated compounds. The term *saturated* is used to describe any organic molecule that contains only single bonds between carbon atoms.

Isomerism in Alkanes

Consider the following structural formulas for butane, C_4H_{10}.



$$\begin{array}{ccccccccc} & H & & H & & H & & H & \\ & | & & | & & | & & | & \\ H- & C & - & C & - & C & - & C & -H \\ & | & & | & & | & & | & \\ & H & & H & & H & & H & \end{array}$$



Note that these two compounds have the same molecular formula, C_4H_{10}, but different structural formulas. Compounds with the same molecular formula but different structural formulas are called *structural isomers*. The two butanes, for which the structural formulas are given above, are isomers of each other. The structural formula containing the straight chain is a *normal* alkane, the other a *branched* alkane.

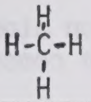
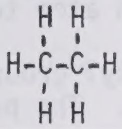
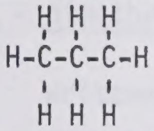
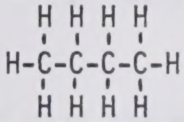
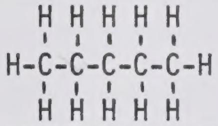
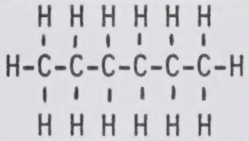
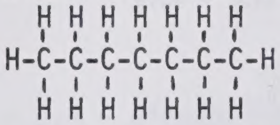
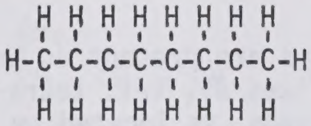
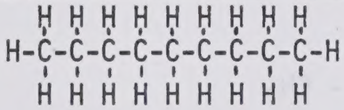
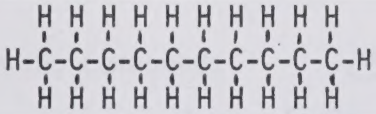
The number of possible isomers increases rapidly as the number of carbon atoms are increased. For example, three isomers are possible for C_5H_{12}, five for C_6H_{14}, 75 for $C_{10}H_{22}$, 366 319 for $C_{20}H_{42}$ and 4 111 846 763 for $C_{30}H_{62}$. Quite obviously, all these isomeric forms, though theoretically possible, have not been prepared. In fact the total number of known organic compounds is less than the number of possible isomers for $C_{30}H_{62}$.

Nomenclature of Alkanes

The large number of isomers poses a major problem of naming organic compounds. This problem is overcome by using a systematic method of nomenclature. (In some instances a common name is retained.) The systematic names, developed by the International Union of Pure and Applied Chemistry (IUPAC), are used by chemists throughout the world. The rules for the nomenclature of alkanes using the IUPAC system are listed below.

1. Continuous chain alkanes are given the name listed in Table H1. Each continuous chain alkane is named according to the stem plus the ending *ane*. The first four members retain the common name and stem. All subsequent stems use the Greek or Latin (non) numerical prefixes.

ORGANIC CHEMISTRY
ALKANES

Name	Molecular Formula	Structural Formula	Phase at Room Temp	Uses
methane	CH_4	 $H-\underset{H}{\overset{H}{C}}-H$	gas	natural gas
ethane	C_2H_6	 $H-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-H$	gas	
propane	C_3H_8	 $H-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-H$	gas	
butane	C_4H_{10}	 $H-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-H$	gas	
pentane	C_5H_{12}	 $H-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-H$	liquid	high grade naphtha gasoline (C_5 to C_{12})
hexane	C_6H_{14}	 $H-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-H$	liquid	
heptane	C_7H_{16}	 $H-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-H$	liquid	
octane	C_8H_{18}	 $H-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-H$	liquid	
nonane	C_9H_{20}	 $H-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-H$	liquid	
decane	$C_{10}H_{22}$	 $H-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-H$	liquid	
	$C_{16}H_{34}$		liquid	kerosene (C_{12} to C_{18}) Lubricating oil mixture of higher hydrocarbons
	$C_{17}H_{36}$		solid	paraffin (C_{20} to C_{30})

Names for Normal (Straight) Chain Alkane Series

Table H1

Note:

Chemists and chemistry students find it very useful to memorize the names (more especially the prefixes) of the first ten alkanes.

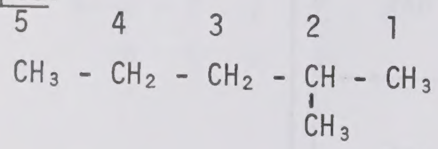
ORGANIC CHEMISTRY

ALKANES

2. The following steps are used in naming branched chain hydrocarbons.

a. Determine the longest continuous chain of carbon atoms in the molecule.
b. Number the carbon atoms of the continuous chain consecutively starting at the end closest to the branching.
c. Locate the branch by the number of the carbon atom to which it is attached on the continuous chain.
d. Name the branch. The branches are called alkyl groups and are named by using the stem of the parent alkane plus the ending *yl*. The position and name of alkyl branches appear first in the final name.

Example:



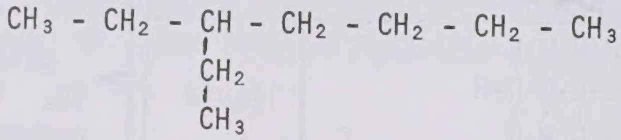
$$\begin{array}{ccccccccc} 5 & & 4 & & 3 & & 2 & & 1 \\ \mathrm{CH_3} & - & \mathrm{CH_2} & - & \mathrm{CH_2} & - & \mathrm{CH} & - & \mathrm{CH_3} \\ & & & & & & | & & \\ & & & & & & \mathrm{CH_3} & & \end{array}$$

2 - methylpentane

location of alkyl branch on chain

branch

longest chain

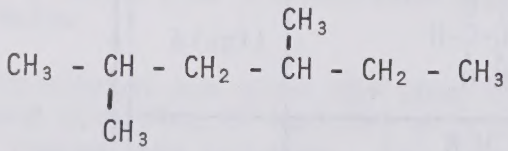


$$\begin{array}{ccccccccccccc} \mathrm{CH_3} & - & \mathrm{CH_2} & - & \mathrm{CH} & - & \mathrm{CH_2} & - & \mathrm{CH_2} & - & \mathrm{CH_2} & - & \mathrm{CH_3} \\ & & & & | & & & & & & & & \\ & & & & \mathrm{CH_2} & & & & & & & & \\ & & & & | & & & & & & & & \\ & & & & \mathrm{CH_3} & & & & & & & & \end{array}$$

3 - ethylheptane

e. If more than one of the same alkyl groups are present as branches, the number of these branches is indicated by the prefixes di, tri, tetra-, penta-, etc. The location of each of these same alkyl groups is located by a number.

Example:

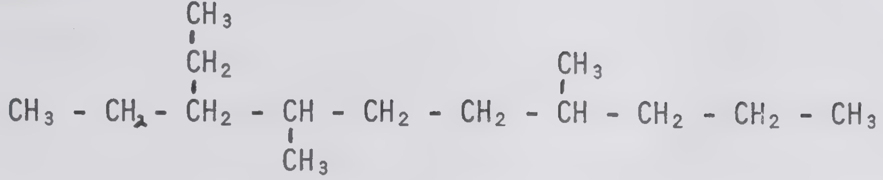


$$\begin{array}{ccccccccccc} & & & & & & \mathrm{CH_3} & & & & \\ & & & & & & | & & & & \\ \mathrm{CH_3} & - & \mathrm{CH} & - & \mathrm{CH_2} & - & \mathrm{CH} & - & \mathrm{CH_2} & - & \mathrm{CH_3} \\ & & | & & & & & & & & \\ & & \mathrm{CH_3} & & & & & & & & \end{array}$$

$$\underbrace{2,\ 4}_{\text{note punctuation}} - \underbrace{\text{dimethylhexane}}_{\text{written as single word}}$$

f. If different alkyl groups are present as branches, assign numbers to locate each branch.

Example:



$$CH_3 - CH_2 - \overset{\begin{matrix}CH_3\\|\\CH_2\\|\end{matrix}}{CH_2} - \underset{\begin{matrix}|\\CH_3\end{matrix}}{CH} - CH_2 - CH_2 - \overset{\begin{matrix}CH_3\\|\end{matrix}}{CH} - CH_2 - CH_2 - CH_3$$

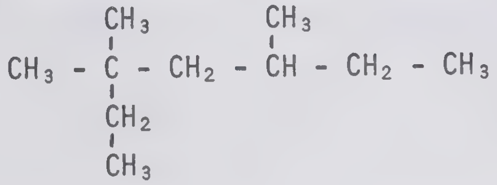
$$\underbrace{3 - ethyl - 4,\ 7,}_{\text{note punctuation}} - \underbrace{dimethyldecane,}_{\text{written as single word}}$$

or, 4, 7 - dimethyl - 3 - ethyldecane

Nomenclature of Alkanes

1. Draw structural formulas and give the names for the five possible isomers of C_6H_{14}.

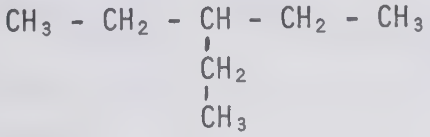
2. Why is the name, 2-ethyl - 2,4 - dimethylhexane unsuitable for the following compound?



$$CH_3 - \underset{\begin{matrix}|\\CH_2\\|\\CH_3\end{matrix}}{\overset{\begin{matrix}CH_3\\|\end{matrix}}{C}} - CH_2 - \overset{\begin{matrix}CH_3\\|\end{matrix}}{CH} - CH_2 - CH_3$$

3. Name each of the following compounds.

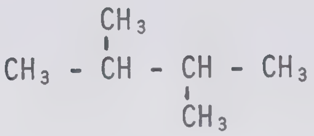
a.



$$CH_3 - CH_2 - \underset{\begin{matrix}|\\CH_2\\|\\CH_3\end{matrix}}{CH} - CH_2 - CH_3$$

____

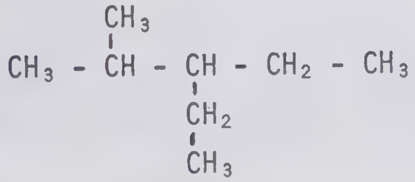
b.



$$CH_3 - \overset{\begin{matrix}CH_3\\|\end{matrix}}{CH} - \underset{\begin{matrix}|\\CH_3\end{matrix}}{CH} - CH_3$$

____

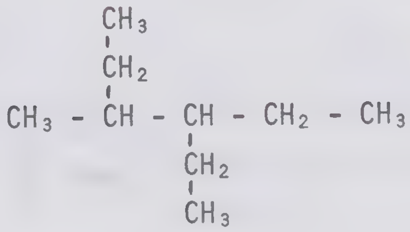
c.



$$CH_3 - \overset{\begin{matrix}CH_3\\|\end{matrix}}{CH} - \underset{\begin{matrix}|\\CH_2\\|\\CH_3\end{matrix}}{CH} - CH_2 - CH_3$$

____

d.

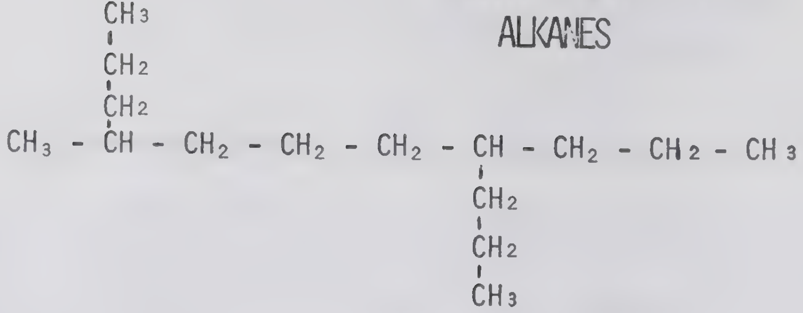


$$CH_3 - \overset{\begin{matrix}CH_3\\|\\CH_2\\|\end{matrix}}{CH} - \underset{\begin{matrix}|\\CH_2\\|\\CH_3\end{matrix}}{CH} - CH_2 - CH_3$$

____

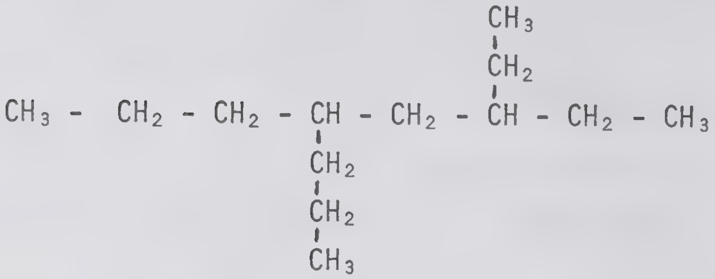
H3, 4

e.



$$\begin{array}{ccccccccccccccccc} & & CH_3 \\ & & | \\ & & CH_2 \\ & & | \\ & & CH_2 \\ & & | \\ CH_3 & - & CH & - & CH_2 & - & CH_2 & - & CH_2 & - & CH & - & CH_2 & - & CH_2 & - & CH_3 \\ & & & & & & & & & & | \\ & & & & & & & & & & CH_2 \\ & & & & & & & & & & | \\ & & & & & & & & & & CH_2 \\ & & & & & & & & & & | \\ & & & & & & & & & & CH_3 \end{array}$$

f.



$$\begin{array}{ccccccccccccccc} & & & & & & & & & & CH_3 \\ & & & & & & & & & & | \\ & & & & & & & & & & CH_2 \\ & & & & & & & & & & | \\ CH_3 & - & CH_2 & - & CH_2 & - & CH & - & CH_2 & - & CH & - & CH_2 & - & CH_3 \\ & & & & & & | \\ & & & & & & CH_2 \\ & & & & & & | \\ & & & & & & CH_2 \\ & & & & & & | \\ & & & & & & CH_3 \end{array}$$

4. Write structural formulas for the following compounds.

a. 3-propylhexane

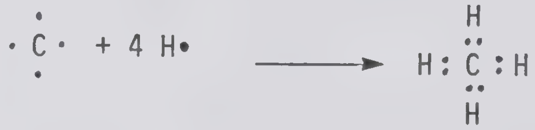
b. 2, 4-dimethylheptane

c. 3, 4-diethyl-3-methylhexane

d. 3-ethyl-4,5-dipropyloctane

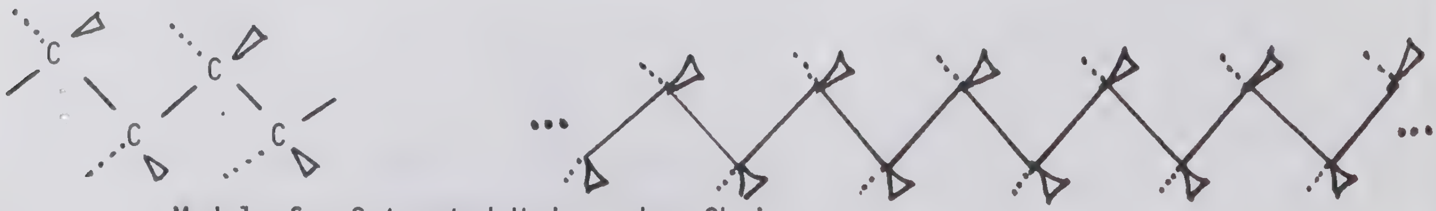
Molecular Shapes of Alkanes

The shape around a carbon atom in an alkane can be predicted from the Lewis diagram of the compound. For example, in methane, CH_4,



$$\cdot\overset{\cdot}{\underset{\cdot}{C}}\cdot + 4\,H\bullet \longrightarrow \begin{array}{ccc} & H & \\ & \cdot\cdot & \\ H: & C & :H \\ & \cdot\cdot & \\ & H & \end{array}$$

Methane has four bonds and zero lone pairs and therefore its shape is tetrahedral. In all saturated hydrocarbons each carbon atom may be represented as having its four covalent bonds directed towards the corners of a tetrahedron. Carbon-carbon single bonds may be considered as two tetrahedra which have a corner in common. A chain of carbon atoms in alkanes can be pictured as a zig-zag arrangement of tetrahedra as shown in Figure H1.



Model of a Saturated Hydrocarbon Chain

Figure H1

ALKANES

Physical Properties of Alkanes

The alkanes form a set of compounds called an homologous series. This is a name applied to any series in which each successive member differs by a CH_2 unit. Within a homologous series (e.g., alkanes) the boiling points (and hence the melting points) increase as the carbon content increases as illustrated in Table H1. This trend is predictable. Molecules of hydrocarbons are nonpolar and it should be expected that von der Waals forces should increase as the number of electrons in the molecule increases. Alkanes containing up to four carbons are gases. The straight chain alkanes from five to sixteen carbon atoms are liquids. Beyond that the compounds are wax-like solids. Further, because alkane intermolecular attractions involve only weak Van der Waals forces, alkanes have relatively low melting and boiling points compared to inorganic compounds of similar molar mass.

Since alkanes are nonpolar, they are not soluble in polar solvents such as water. Liquid alkanes are good solvents for other hydrocarbons.

Chemical Properties of Alkanes

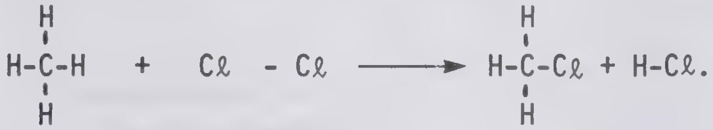
Alkanes are relatively unreactive under ordinary conditions. However, some reactions of alkanes are common at higher temperatures.

1. Alkanes react with oxygen (burn or undergo combustion) at high temperatures to produce primarily CO_2 and H_2O. The reaction is called combustion. Alkanes used in this manner are called fuels. For example, the burning of propane is represented by the equation,

$$C_3H_8 + 5O_2 \longrightarrow 3CO_2 + 4H_2O.$$

2. In the absence of air, alkanes can be *cracked* (broken into smaller fragments) at high temperatures or in the presence of catalysts. This process is called *catalytic cracking*. The cracking reaction is commonly used to convert high molar mass hydrocarbons (C_{15} to C_{18}) to gasoline hydrocarbons (C_5 to C_{12}).

3. Alkanes can undergo substitution reactions in which another atom or group of atoms is substituted for a hydrogen atom. For example, the chloro substitutions of methane can be represented by the equation,



$$\mathrm{H{-}\underset{H}{\overset{H}{C}}{-}H} + \mathrm{C\ell - C\ell} \longrightarrow \mathrm{H{-}\underset{H}{\overset{H}{C}}{-}C\ell} + \mathrm{H{-}C\ell}.$$

Substitutions reactions of alkanes usually occur very slowly and only in the presence of light.

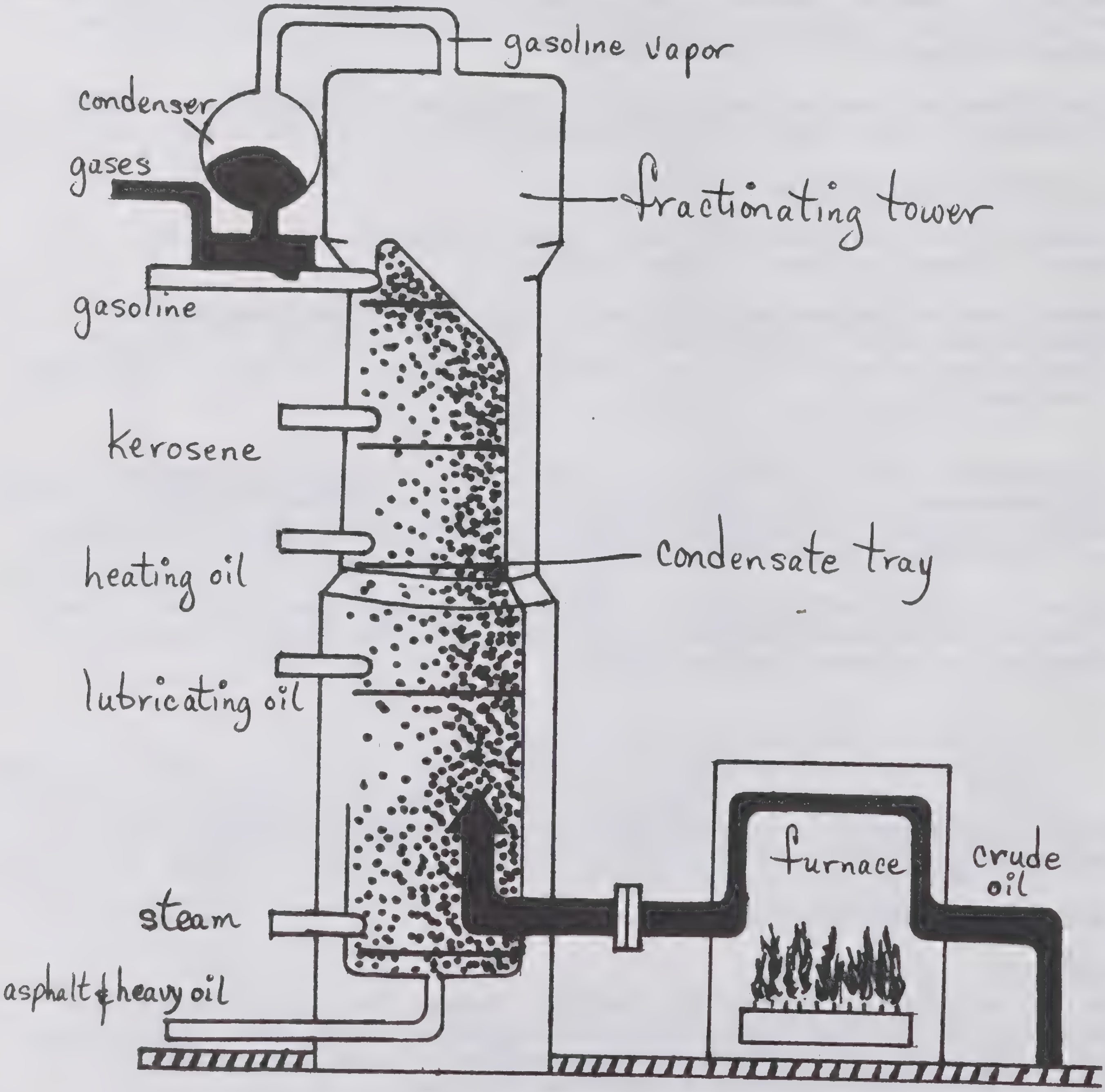
Some Common Sources and Uses of Alkanes

1. Petroleum

The main source of hydrocarbons is petroleum. However, the various hydrocarbon components of crude petroleum must be separated before they can be used. The processes involved in separation, purification and increasing the yield of the desireable components of crude petroleum is called *petroleum refining*.

Since crude petroleum is a complex mixture of hydrocarbons, it has no fixed boiling point. The mixture has a boiling or distillation range which may start as low as 20°C and end above 400°C. The difference in the volatility or boiling point of components or fractions in the mixture makes possible the initial rough separation of crude petroleum by *fractional distillation or fractionation*.* In general, the smaller the molecule the lower its boiling point, (recall the variation of van der Waals forces with number of electrons in the molecule). As a result fractional distillation sorts the crude petroleum into its main constituents according to the size of molecules.

The separation of crude petroleum by fractional distillation is affected in vertical columns containing series of horizontal plates or trays (see Figure H2). The crude petroleum is heated to about 400°C and the vapors pass into the fractionation tower.



Schematic Diagram of a Typical Modern Fractionation Tower

Figure H2

---

* Other processes involved in petroleum refining include purification by solvent extraction, absorption, crystallization, catalytic cracking and catalytic reforming.

As the vapors pass through the openings in the trays they condense to the liquid phase. The more volatile portion of the liquid re-vaporizes and rises to the next tray. The less volatile portion remains on the tray where it serves to condense new vapors rising from below. Thus, the various fractions of the crude oil distribute themselves among the trays according to boiling temperature ranges. In this way, the extremely light gases are taken off at the top of the tower, gasoline from the top reaction, the kerosine and gas oils in the middle, and the lubricants, waxes and fuel oils at the bottom. Residue drawn off at the bottom may be burned as fuel, processed into asphalt, or heated further to produce other hydrocarbons and a residue of coke (See Table H2).

Fractional distillation is a physical process, and does not alter the composition of the hydrocarbon molecules. To bring about chemical changes, other refining methods are used, generally called *cracking or reforming processes.*

The first cracking processes, because of the use of high temperatures, were called *thermal cracking*. These have been largely replaced by methods called catalytic cracking in which the molecular breakdown is brought about by catalysts. The cracking process breaks down large molecules into smaller molecules; e.g. heavier fractions are broken down into more useful fractions such as gasoline or kerosine.

Thermal and catalytic reforming uses heat or catalysts respectively to convert lighter molecules into heavier fractions. Reforming is most commonly used to convert low-grade gasolines into higher-grade fuels, and to produce hydrocarbons for chemical use.

By using fractional distillation and various other processes, the end-products from refining can be varied within fairly wide limits. Generally, the main factors which affect the end-products are the kind of crude petroleum available (crudes from different sources may vary in their constituents) and the economic demands for specific products.

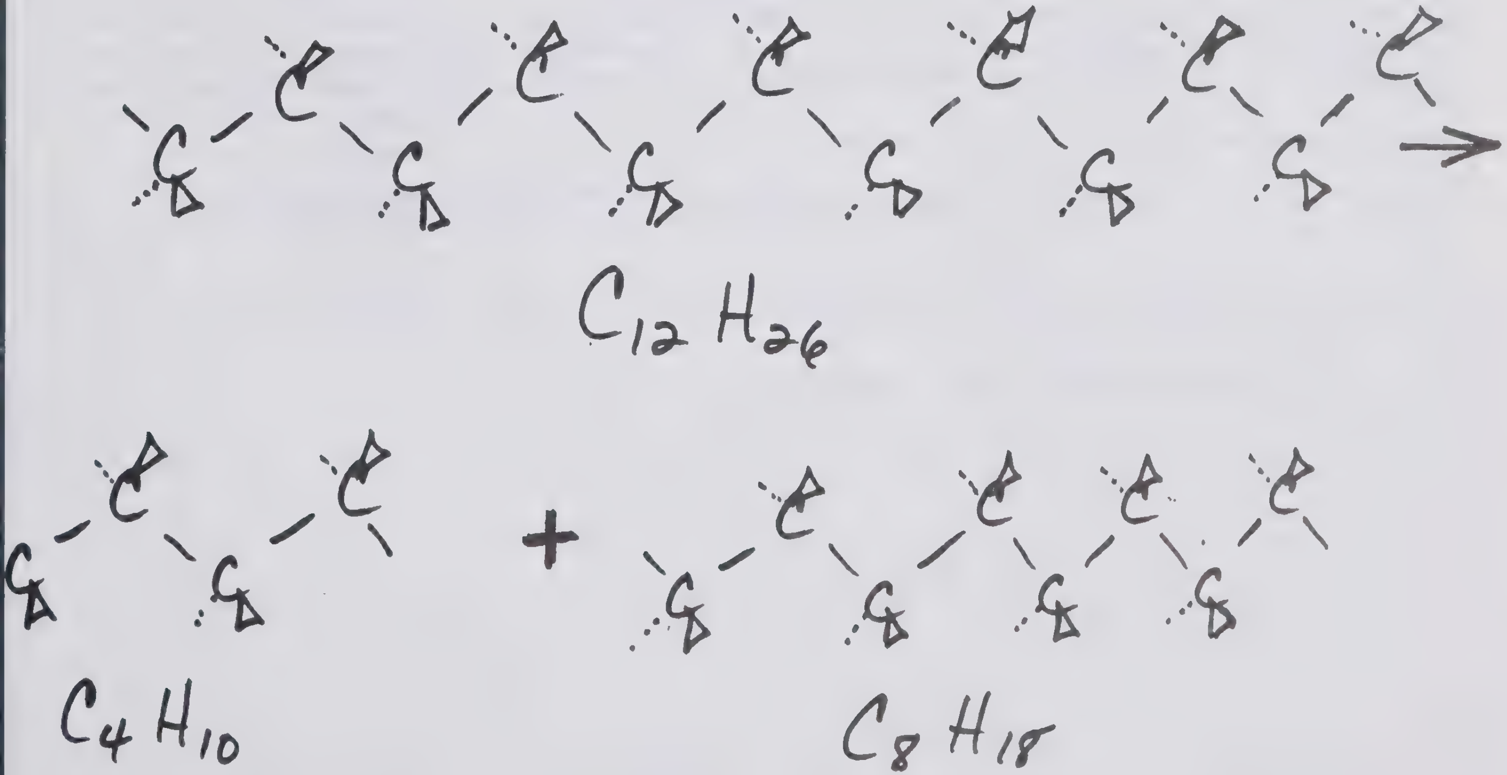


Table H2

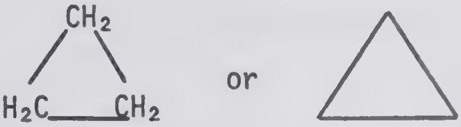
Fractions from the fractional Distillation of Petroleum

Range of Carbon Atoms	Boiling Point Range (^{o}C)	Fraction	Some Typical Uses
C_1- C_5*	-164 to 30	gas	gaseous fuel; e.g., heating homes
C_5 - C_{17}	30 to 90	petroleum ether	solvent, drycleaning
C_5 - C_{12}	30 to 200	straight-run gasoline	motor gasoline
C_{12} - C_{16}	175 to 275	kerosene	fuel for stoves, diesel and jet engines; cracking stock
C_{15} - C_{18}	up to 375	light gas oil or fuel oil	furnace oil; cracking stock
C_{16} - C_{20}	350 and up	heavy gas oil	lubricating oils; cracking stock
C_{18} - up	semi solid	greases	lubrication; cracking stock
C_{20} - up	melts at 52 - 57	paraffin (wax)	candles, waxed paper, cosmetics, polishes; cracking stock
C_{26} - up	to 515^{o}C	residue in boiler	asphalts and tars (roofing and paving; wax; residual oils)

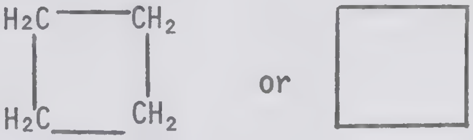
* Also obtainable from natural gas

Cycloalkanes

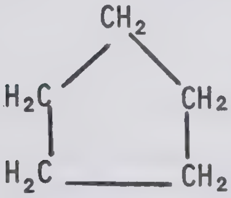
Compounds containing rings of saturated carbon atoms are known as cycloalkanes. For convenience, cyclic hydrocarbons can be represented by simple geometric figures: a triangle for a three-carbon ring, a square for a four-carbon ring, etc. It must be remembered that each carbon still possesses four bonds. In structural diagrams hydrogen is assumed to be bonded to carbon to satisfy carbon's bonding capacity unless some other substituent is indicated. Note that a cyclic compound contains two less hydrogen atoms than the noncyclic compound with the same number of carbon atoms. Thus the general formula for cycloalkanes is C_nH_{2n}. The following examples illustrate the nomenclature, molecular formulas and structural formulas for cycloalkanes.



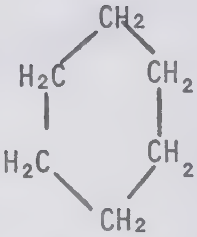
cyclopropane, C_3H_6



cyclobutane, C_4H_8

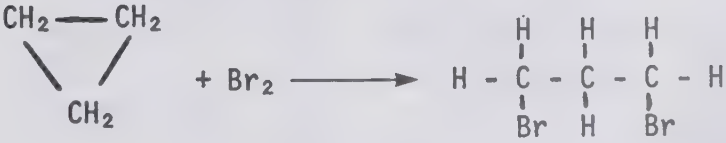


cyclopentane, C_5H_{10}



cyclohexane, C_6H_{12}

The cycloalkanes have higher boiling points and densities than the corresponding alkanes because of their more compact structure. Their chemical properties are similar to those of the alkanes except that the small ring compound's (up to 5 carbons) are) are more reactive. This is because the C-C-C in the small rings are considerably less than the tetrahedral angle, resulting in a strained structure. Cycloalkanes react by allowing the ring to open and to undergo addition reactions as illustrated by the following reaction.



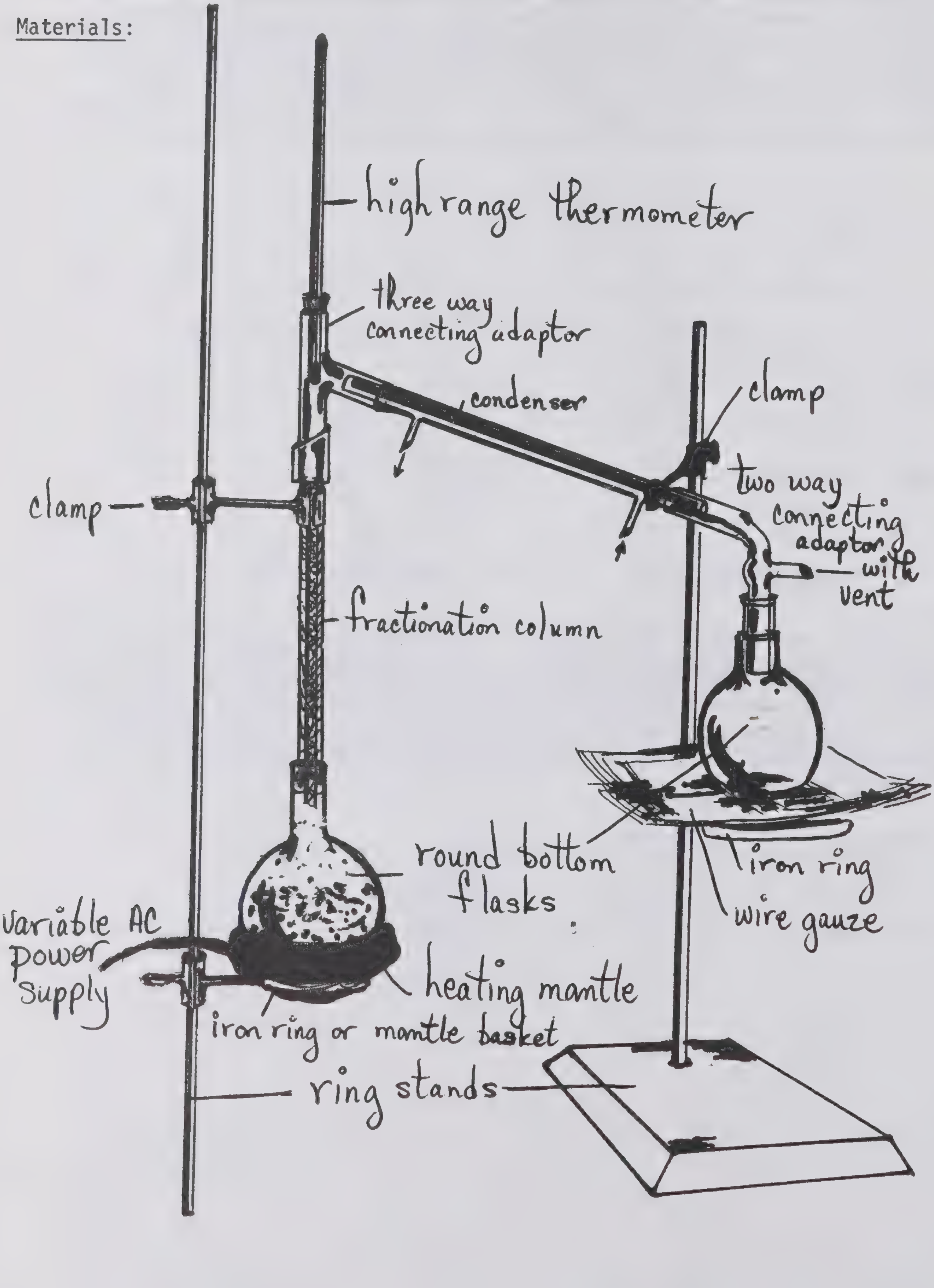
ORGANIC CHEMISTRY

FRACTIONAL DISTILLATION - DEMO H1

Purpose:

To separate a two-component mixture by the method of fractional distillation.

Materials:



H 12a

FRACTIONAL DISTILLATION OF A TWO COMPONENT MIXTURE

Temperature (°C)

Time (minutes)

ORGANIC CHEMISTRY

FRACTIONAL DISTILLATION - DEMO H1

Procedure:

1. Assemble the apparatus as pictured.
2. Place 50 ml of the mixture in the distillation flask. Add several boiling chips.
3. Check to ensure that all connections are tight.
4. Heat the mixture slowly.
5. When the temperature starts to rise, record the temperature every 30 seconds.

   Note: The levelling-off of temperature indicates that one of the components of the mixture is boiling. At this temperature liquid will begin to collect in the collection flask.

6. Once the temperature begins to rise again, change the collection flask to collect the next component that distills.
7. Continue heating until the temperature levels off again. Continue the procedure only until a few ml remains in the heating flask. Do not heat to dryness.
8. Use the 25 ml graduated cylinder to measure the volume of the first fraction collected. Record this volume in the data table provided and calculate the volume of the second fraction by subtraction.
9. Plot a graph of temperature versus time on the ruled page provided.
10. From the graph plotted, determine the temperature that most likely represents the boiling point of each component. Record these temperatures in the data table provided.
11. Calculate the percent composition of the mixture. Record this composition in the data table provided, Show your work.

Observations and Calculations:

Fraction	Boiling Point	Volume	Percent by Volume (Show Method)
I			
II		(by subtraction)	

Questions:

1. Account for the plateaus on the graph of temperature versus time.

2. Account for the relatively rapid rise in temperature between the plateaus on the graph of temperature versus time.

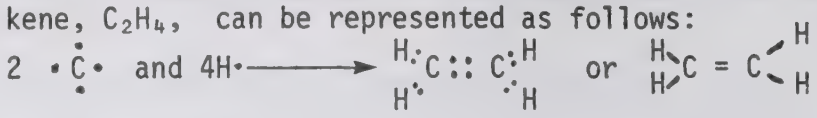
3. Account for the large difference in boiling point between hexane and hexanol.

H3, 4

ALKENES

Bonding in Alkenes

The alkenes (general formula - C_nH_{2n}) contain two less hydrogen atoms than the alkanes with the same number of carbon atoms. Since each carbon must have four covalent bonds, the lower H-to-C ratio necessitates that a double bond be placed between one pair of carbon atoms. Because of the presence of a double bond, the term *unsaturated* is applied to the compounds in this series. Each carbon atom that is part of the double bond in an alkene is bonded to two other atoms. For example, the bonding in the simplest alkene, C_2H_4, can be represented as follows:



Nomenclature of Alkenes

The IUPAC system of nomenclature for the alkanes applies to the alkenes with the following additions.

a. The ending *ene* is used (instead of ane) to indicate the presence of one carbon-to-carbon double bond.

b. The longest continuous chain of carbon atoms *containing the double bond* determines the stem for the name.

c. The longest continuous chain is numbered so that the carbon atoms of the double bond have the lowest possible numbers.

The common names for some of the lower chain alkenes is still often used. The examples following give the IUPAC names as well as the common name (in brackets) for the first two members.

$CH_2 = CH_2$

ethene (ethylene)

(to make polyethene)

$CH_2 = CH - CH_3$

propene (propylene)

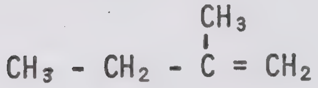
(to make polypropene)

$CH_2 = CH\text{-}CH_2 - CH_3$

1 - butene

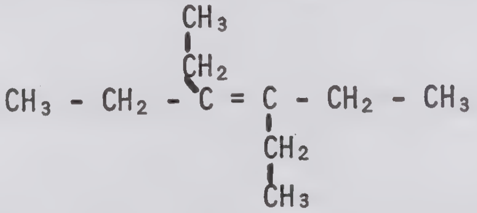
$CH_3 - CH = CH - CH_3$

2 - butene



$CH_3 - CH_2 - \overset{\overset{CH_3}{|}}{C} = CH_2$

2 - methyl-1-butene



$CH_3 - CH_2 - \overset{\overset{CH_3}{|}}{\overset{CH_2}{|}}{C} = \underset{\underset{CH_3}{|}}{\underset{CH_2}{|}}{C} - CH_2 - CH_3$

3, 4-diethyl - 3-hexene

(Note: that cycloalkanes - general formula CnH_2n) are isomeric with alkenes - general formula C_nH_{2n}.)

ORGANIC CHEMISTRY

ALKENES

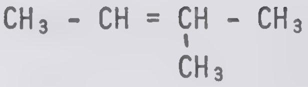
Names and Structural Formulas of Alkenes

1. Give the name for each of the following compounds.

a. $CH_3 - CH_2 - CH_2 - CH = CH - CH_3$

____

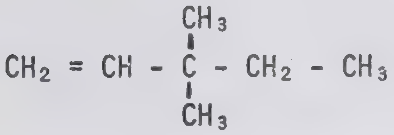
b.



$CH_3 - CH = \underset{\substack{|\\ CH_3}}{CH} - CH_3$

____

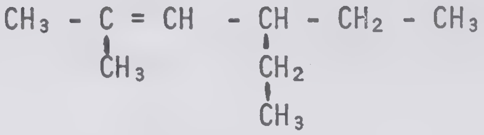
c.



$CH_2 = CH - \overset{\substack{CH_3\\ |}}{\underset{\substack{|\\ CH_3}}{C}} - CH_2 - CH_3$

____

d.



$CH_3 - \underset{\substack{|\\ CH_3}}{C} = CH - \underset{\substack{|\\ CH_2\\ |\\ CH_3}}{CH} - CH_2 - CH_3$

____

2. Write a structural formula for each of the following compounds.

a. 3-octene

b. 2, 4 - dimethyl - 2 - pentene

c. 4-ethyl - 3-methyl - 2-hexene

d. a cyclic hydrocarbon isomeric with 1-hexene

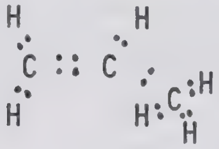
3. Draw structural formulas for 6 isomeric forms of C_5H_{10}. (Note: give one isomeric form as a cyclic hydrocarbon).

ORGANIC CHEMISTRY

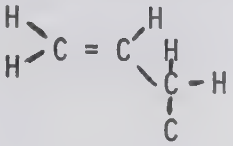
ALKENES

Shapes of Alkenes

The shape of propene can be determined from the Lewis electron-dot diagram.



or



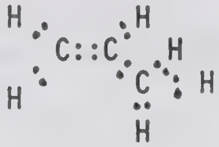
Remembering that multiple bonds are counted as single bonds for purposes of predicting shape. It will be observed that three bonds and zero lone pairs surrounds each of the double bond carbons. Thus the shape around the carbons with a double bond is trigonal planar. The shape around each of the saturated carbons is tetrahedral.

Physical Properties of Alkenes

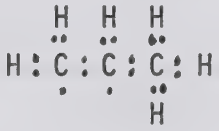
The physical properties of alkenes roughly correspond to the physical properties of alkenes with the same number of carbons. Refer back to the physical properties of alkanes discussed earlier.

Chemical Properties of Alkenes

1. Alkenes (like alkanes) react with oxygen (burn or undergo combustion) at high temperatures to produce primarily CO_2 and H_2O.
2. Alkenes are chemically more reactive than alkanes because of their ability to undergo addition reactions at the site of the double bond. Only a single bond is necessary to hold the molecule together. The second pair of electrons in the double bond of the alkene is available for reaction under the right conditions. For example,

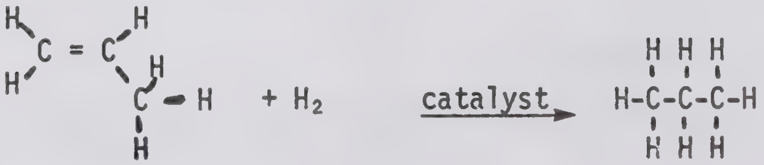


can become

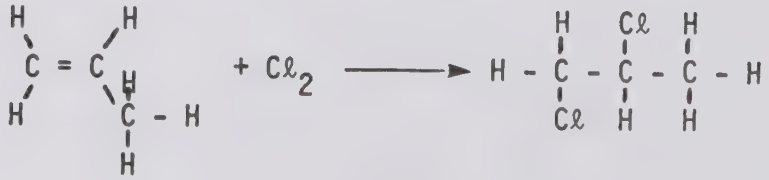


which makes available two bonding electrons. The reaction is called an *addition reaction* because atoms of some substance can be added to the alkene. Some examples of addition reactions are given below.

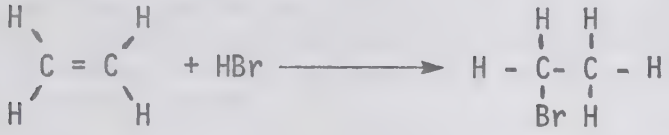
a. addition reactions with hydrogen



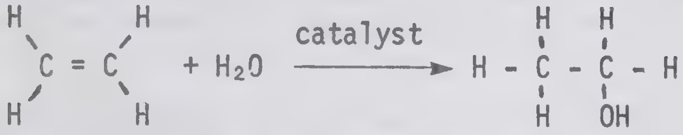
b. addition reactions with a halogen



c. addition reactions with a hydrogen halide



d. addition reactions with water



Note: that in all instances the double bond is eliminated and a saturated compound is formed.

3. Oxidizing agents such as $KMnO_4$ and $K_2Cr_2O_7$ also readily react with alkenes by attaching at the site of the double bond. For example, when potassium permanganate is added to an unsaturated hydrocarbon, the violet color of permanganate fades. (This reaction, as well as the reaction with bromine, is used as a test for the presence of unsaturation in hydrocarbons.)

Some Sources and Uses of Alkenes

Alkenes are usually obtained in industrial quantities by the catalytic cracking of alkanes. (Recall that catalytic cracking is a process by which longer chain molecules are broken down into shorter chain molecules.) The shorter chain alkenes (up to 5 carbon atoms) can be obtained from the fractional distillation of petroleum. Higher chain alkenes, which cannot be separated from petroleum, remain as valuable components of gasoline.

Alkenes, particularily ethene (ethylene), because of their unsaturation and consequent chemical reactivity, serve as starting materials for a vast variety of useful organic compounds. (In Alberta, the production and utilization of ethene is expected to become a major petrochemical industry.) Only a few of the many useful products derived from ethene will be considered here.

a. Manufacture of plastics and synthetic fibres.

Under proper conditions, ethene can react with itself to form a polymer known as polyethene (polyethylene). Polyethene is a very long chain hydrocarbon formed by the joining of 500-700 ethene units.

$$nCH_1 = CH_2 \longrightarrow \left(CH_2 - CH_2 \right)_n$$

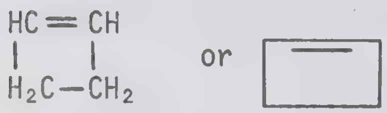
The use of polyethene is as varied as for any single substance known - including chemical equipment, packaging material, industrial protective, clothing and toys. The manufacture of various other plastics and synthetic fibres use ethene as a starting material. The usefulness of polyethene and other polymers is unquestionable. However, at the same time, their use poses an environmental hazard, since most of these plastics are not biodegradeable. Thus the utility of plastics and the consequence of their continued use pose a dilemma in modern society.

(The process of forming huge, high molar mass molecules from smaller molecules is called *polymerization.* The large molecule, or unit is called the *polymer* and the small unit the *monomer.* The term polymer has its origin from the Greek word *poly,* meaning *many* and *meres* meaning *part.* For example, ethene is a monomer and polyethene is a polymer.)

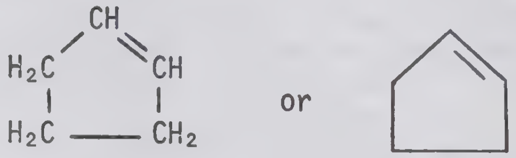
b. Ethylene is used as a starting compound in the manufacture of other common products such as DDT (insecticide), synthetic detergents, ethylene glycol (antifreeze), ethylene chloride and tetraethylead (antiknock agents in gasoline), paints and drugs.

Cycloalkenes

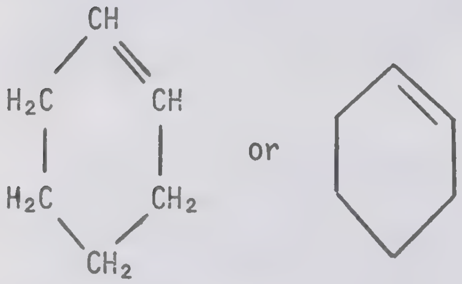
Alkenes consisting of a closed ring structure are known as cycloalkenes. As with cycloalkanes, the stem name for cyclic alkenes is the same as that for the corresponding straight chain alkenes. The name for the cycolalkene as for the cycloalkane is preceded by the prefix cyclo. The cycloalkenes have two less hydrogens than the corresponding alkene, hence their general formula is C_nH_{2n-2}. The following examples illustrate the nomenclature, molecular formulas and structural formulas for cycloalkenes.



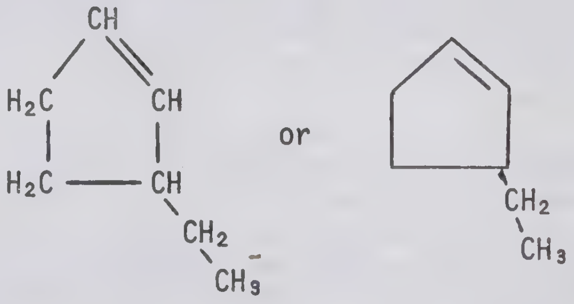
C_4H_6, cyclobutene



C_5H_8, cyclopentene



C_6H_{10}, cyclohexene



C_7H_{12}, 3-ethylcyclopentene

The cycloalkenes have slightly higher boiling points and densities than the alkenes containing the same number of carbon atoms. Their chemical properties are similar to those of the alkenes except that the small ring compounds are more reactive than the corresponding alkene. The reason for this was given earlier when the reactivities of cycloalkenes and alkanes was compared.

Bonding in Alkynes

Alkynes are hydrocarbons that contain a triple bond between one pair of carbon atoms. The alkynes contain two less hydrogens than the corresponding alkene (or four less than the corresponding alkane), hence the general formula for alkynes is C_nH_{2n-2}. The alkynes, like the alkenes are called unsaturated because they each contain a multiple bond.

ORGANIC CHEMISTRY

ALKYNES

Each carbon atom that is part of the triple bond in an alkyne is bonded to one other atom. The bonding in the simplest alkyne, C_2H_2, can be represented as follows:

$2 \cdot \overset{\cdot}{\underset{\cdot}{C}} \cdot$ and $2H\cdot \longrightarrow H{:}C{:}{:}{:}C{:}H$ or $H\text{-}C\equiv C\text{-}H$

Nomenclature of Alkynes

The IUPAC nomenclature for the alkynes is identical to that of the alkenes except the ending *yne* is used to indicate the presence of a triple bond. The names (including the common name for the first member) and the structural formulas for some of the representative members of the series are given in the examples following.

$H\text{-}C\equiv C\text{-}H$
ethyne (acetylene)

$HC\equiv C\text{-}CH_3$
propyne

$HC\equiv C\text{-}CH_2\text{ -}CH_3$
1-butyne

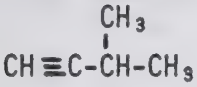
$H_2C\text{-}C\equiv C\text{-}CH_3$
2-butyne

Note that the cycloalkenes - general formula, CnH_2n_{-2} are isomeric with alkynes - general formula, C_nH_{2n-2}.

Names and Structural Formulas of Alkynes

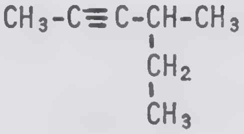
1. Give the name for each of the following compounds?

a.



$CH\equiv C\text{-}\overset{\overset{CH_3}{|}}{C}H\text{-}CH_3$

b.



$CH_3\text{-}C\equiv C\text{-}\underset{\substack{|\\CH_2\\|\\CH_3}}{C}H\text{-}CH_3$

2. Write a structural formula for each of the following compounds.

a. 4, 4-diethyl-1-hexyne

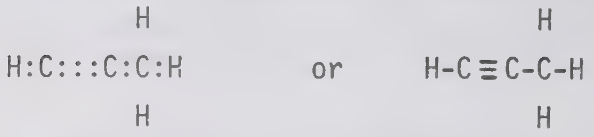
b. 5-ethyl-4-propyl-2-heptyne

3. Give the structural formula and names for three isomeric forms of C_4H_6. One of the isomeric forms is a cycloalkene.)

ALKYNES

Shapes of Alkynes

The shape of propyne can be determined from the Lewis electron dot diagram.



$$H{:}C{:}{:}{:}C{:}\overset{H}{\underset{H}{C}}{:}H \quad \text{or} \quad H-C\equiv C-\overset{H}{\underset{H}{C}}-H$$

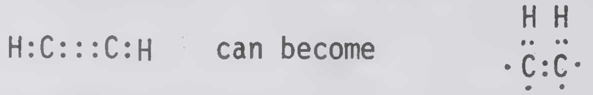
Multiple bonds are counted as single bonds for purposes of predicting shape. It should be noted that two bonds and zero lone pairs surrounds each of the carbon atoms involved in the triple bond and therefore the shape around their carbons is linear. The shape around each of the saturated carbons is still tetrahedral.

Physical Properties of Alkynes

The physical properties of alkynes are quite similar to the physical properties of alkenes and alkanes with corresponding number of carbon atoms. Refer back to the discussion of properties of alkanes as a review of the typical physical properties.

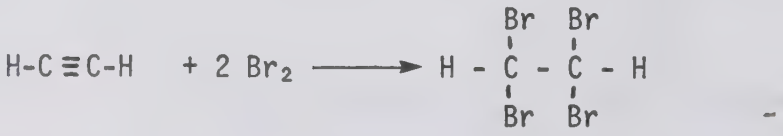
Chemical Properties of Alkynes

1. Alkynes (like alkenes and alkanes) can react with oxygen (burn or undergo combustion) at high temperatures to produce mainly CO_2 and H_2O. (Acetylene is an important example.)
2. Alkynes, similar to the alkenes, can undergo addition reactions. In this respect, the alkynes are even more reactive than the alkenes since they can make available four bonding electrons, as shown below:



$$H{:}C{:}{:}{:}C{:}H \quad \text{can become} \quad \cdot\overset{H}{\underset{\cdot}{\ddot{C}}}{:}\overset{H}{\underset{\cdot}{\ddot{C}}}\cdot$$

Alkynes can undergo addition at four sites, as illustrated in the examples following.

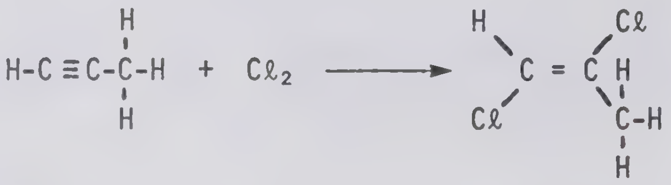


$$H-C\equiv C-H \quad + 2\,Br_2 \longrightarrow H-\overset{Br}{\underset{Br}{C}}-\overset{Br}{\underset{Br}{C}}-H$$

1,1,2,2-tetrabromoethane

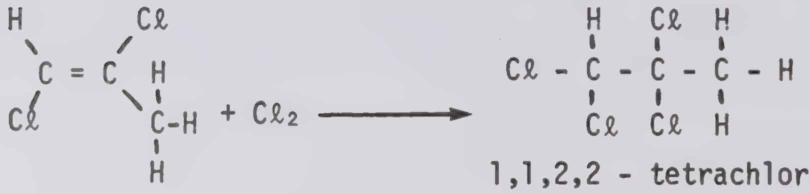
The addition reaction can probably proceed in two ways, depending upon the availability of added reagent, as the following examples show.

Step 1:



1, 2-dichloropropene

Step 2:



1,1,2,2 - tetrachloropropane

Some Sources and Uses of Alkynes

Ethyne, the most useful alkyne, is prepared commercially in large quantities. It can be prepared by reacting water with calcium carbide, but is prepared mainly by cracking methane at the high temperatures of an electric arc.

$$2CH_4 \xrightarrow[\text{electricity}]{\text{heat}} C_2H_2 + 3H_2$$

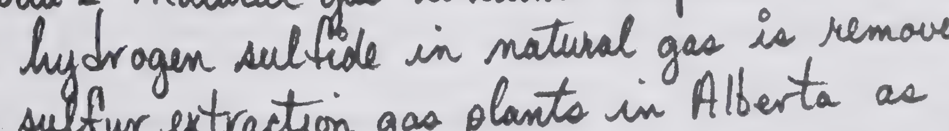
Ethyne is so unsaturated that it reacts with many substances, including hydrogen, halogen acids ($HC\ell(aq)$ and $HC\ell O_3(aq)$), and other alkynes. Thus ethyne is an excellent starting material for the commercial synthesis of more complex organic compounds such as ethanoic acid, ethyl and other alcohols, benzene, synthetic rubber and synthetic fibers such as Orlon, Acrilan and Dynel. The polymerization of ethyne, like that of ethene, represents a typical reaction of unsaturated hydrocarbons. The high heat of combustion of ethyne also makes it useful in *oxy-acetylene* welding. The large amounts of heat are provided by the following reaction:

$$2C_2H_2 + 5O_2 \longrightarrow 4CO_2 + 2H_2O + \text{heat}$$

(It should be noted that ethyne is really the only unsaturated hydrocarbon that is burned as a fuel or source of heat.)

Alberta's Petrochemical Industry

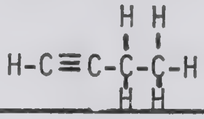
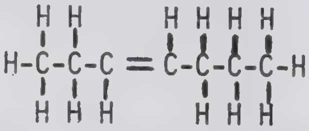
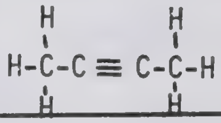
Alberta's natural gas contains compounds other than methane. The hydrogen sulfide in natural gas is removed by the over 30 sulfur extraction gas plants in Alberta as elemental sulfur. The LP (liquid petroleum) gas are removed by four gas liquification plants in Alberta. The LP gases include butane, propane and ethane. Ethane has been of lesser importance but now will become the most important of these gases. After the ethane is removed from natural gas by cooling and compression it is "cracked" by heat into ethene – the main building block of Alberta's coming petrochemical industry.



Alberta Gas Ethylene (AGE) in Red Deer will by 1980 produce 0.55 million tonnes per year of ethene. Of this amount 0.32 million tonnes will be consumed in Alberta.

ORGANIC CHEMISTRY

ALKANES, ALKENES, ALKYNES

	Name	Molecular Formula	Structural Formula
1.	2-hexene		
2.			 $H-C\equiv C-\overset{H}{\underset{H}{C}}-\overset{H}{\underset{H}{C}}-H$
3.		C_5H_{12}	
4.			 $H-\overset{H}{\underset{H}{C}}-\overset{H}{\underset{H}{C}}-\underset{H}{C}=\overset{H}{C}-\overset{H}{\underset{H}{C}}-\overset{H}{\underset{H}{C}}-\overset{H}{\underset{H}{C}}-H$
5.		C_3H_6	
6.	ethyne		
7.	propane		
8.		C_3H_4	
9.			 $H-\overset{H}{\underset{H}{C}}-C\equiv C-\overset{H}{\underset{H}{C}}-H$
10.	2-pentene		

11. Determine the shape around a carbon atom in ethane.

12. Determine the shape around carbon number 2 in the compound 1-butene.

13. Determine the shape around carbon number 3 in the compound 2-pentyne.

14. How many electrons are shared by the carbon atoms that are part of a carbon-carbon triple bond?

MOLECULAR MODELS OF ALKANES AND ALKENES - LAB H1

Purpose: To construct models for some alkanes and alkenes.

Procedure:

Part A:

1. Obtain a molecular model kit. An accompanying instruction sheet lists the color code for the balls. A ball represents one atom and a spring represents one covalent bond.
2. Start with a model of methane, CH_4. Record the structural formula in Table H1.
3. Replace one hydrogen atom in methane with another carbon atom and add as many hydrogen atoms as the additional carbon atoms can accommodate to satisfy the bonding capacity of every carbon.
4. Repeat step three by successively replacing an additional hydrogen atom with a carbon atom, then adding the required number of hydrogen atoms until Table H1 information has been completed. Note that some members can assume different structures.

Part B:

1. From the molecular model kit used in Part A procedure, select two carbon atoms and connect them using two springs. Complete the model by adding the required number of hydrogen atoms. This model represents a molecule of the first member of the alkene series, ethene or ethylene. Record the structural formula in Table H2.
2. Note that the carbon atoms about the double bond are not free to rotate.
3. Replace one hydrogen atom in ethene with another carbon atom and add the required number of hydrogen atoms to form the second member of the alkene series. Record the information relating to this structure in Table H2.
4. Replace a hydrogen atom that is on the singly bonded carbon and add the required number of hydrogen atoms to form a third member of the alkene series. Record these structures in Table H2.
5. Construct another model of the third member of the alkene series in which the double bond occurs in the middle rather than next to an end carbon. Compare this model with the model constructed in Step 4 above. Record this structure in Table H2.
6. (Optional) Construct a different model of the third member of the alkene series in which the double bond occurs in the middle. Compare this model to the one constructed in Step 5. Record this structure in Table H2.

ORGANIC CHEMISTRY

H3, 4

MOLECULAR MODELS OF ALKANES AND ALKENES

TABLE H1

Alkanes

Member	Molecular Formula	Structural Formula	Name
First			
Second			
Third			
Fourth			
Fifth			

ORGANIC CHEMISTRY
MOLECULAR MODELS OF ALKANES AND ALKENES - LAB H1
TABLE H2

H3, 4

ALKENES

Member	Molecular Formula	Structural Formula	Name
First			
Second			
Third			

Questions:

Part A:

1. For each carbon atom added, the number of hydrogen atoms added is ______ Each successive member of the alkane series differs from the preceeding member by a unit whose formula is ______ .
2. The fourth and fifth members of the alkane series have more than one structural formula. Compounds with the same molecular formula but different structural formulae are called ______ .
3. Since carbon forms only one bond with an adjacent carbon for each member in the alkane series, the bonding in the alkane series is said to be ______ .

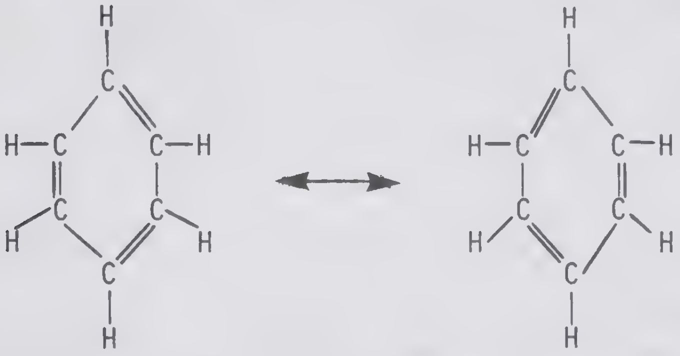
Part B:

4. The successive members of the alkane series differs from a preceeding member by a common unit whose formula is ______ .
5. (Optional) Draw structural formulas for five noncyclic forms of C_5H_{10}.

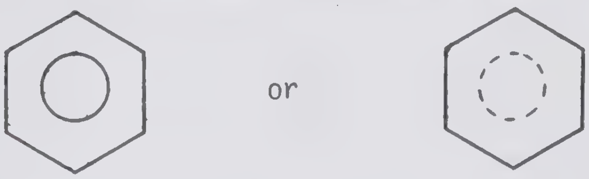
ORGANIC CHEMISTRY
AROMATICS

Bonding in Aromatics

The parent molecule of aromatic compounds is benzene, C_6H_6. The six carbon atoms in benzene are arranged in a cyclic structure, with one hydrogen atom attached to each carbon atom. The structure can be represented by the following diagrams, with alternate single and double bonds between carbon atoms.



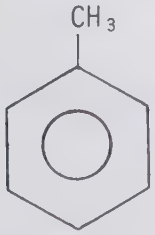
However, since evidence indicates that all bonds between the carbon atoms are equivalent, neither a single nor a double bond is present. The actual structure is a hybrid of the two structures shown above. The valence electrons are evenly distributed over the entire ring. The benzene structure is conventionally represented as



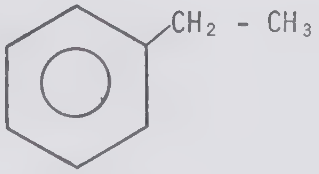
where the circle represents the evenly distributed electrons. It is understood that at each point in the hexagon there exists a carbon atom with one hydrogen atom bonded to it.

Nomenclature of Aromatics

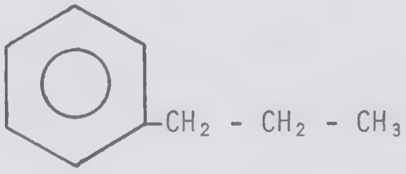
A great variety of substituted benzenes are known with one or more of the hydrogen atoms of the ring replaced by other atoms or groups. For present purposes, consideration is being limited to substituted benzene compounds, where one or more hydrogen atoms has been replaced by only one or more alkyl groups. (Alkyl groups correspond to the alkane hydrocarbons, but have one hydrogen atom less, e. g., -- CH_3 is a methyl group.) According to the IUPAC system, the alkyl monosubstituted aromatic compounds are named as alkylbenzenes, although in some instances the trivial name persists. The formulas and names for several alkyl monosubstituted benzene compounds are shown below.



methylbenzene
(toluene)



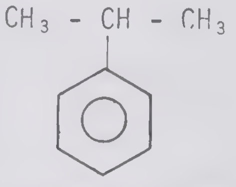
ethylbenzene



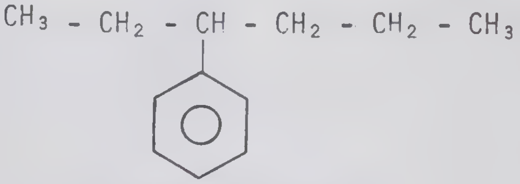
propylbenzene

Note that it does not matter which carbon atom the group is attached to because all of the carbon atoms in benzene are equivalent.

In those compounds in which the alkyl substituent is attached to the benzene ring by other than an end carbon, it is more convenient to consider the benzene ring as a branch. In this case, the benzene ring with one hydrogen atom less; i. e., C_6H_5-, is called a phenyl group. The following examples illustrate this point.

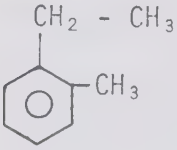


2-phenylpropane

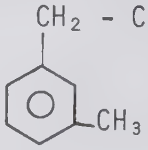


3-phenylhexane

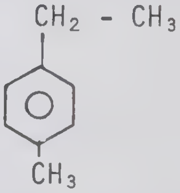
When two hydrogen atoms of benzene are replaced, the replacing groups can be arranged so as to give three isomers. These compounds are named as disubstituted benzenes, with the group positions indicated by numbers or by the names *ortho*, symbolized *o*, (groups on adjacent carbon atoms); *meta*, symbolized *m*, (one carbon between groups); and *para*, symbolized *p*, (two carbons between groups). These arrangements, where methyl and ethyl groups have been added, are shown in the examples below.



2-methylethylbenzene, or
o-methylethylbenzene
(also, *o*-ethyltoluene)

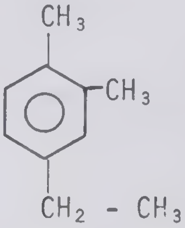


3-methylethylbenzene, or
m-methylethylbenzene
(also, *m*-ethyltoluene)

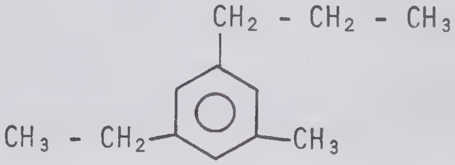


4-methylethylbenzene,
p-methylethylbenzene
(also, *p*-ethyltoluene)

When three or more hydrogen atoms of benzene are replaced, the carbon atoms in the ring are given numbers which indicate the positions of the substituting groups. The starting point for numbering is the carbon to which the largest group is attached. The following examples will help to clarify this idea.



1-ethyl-3, 4-dimethylbenzene,
3, 4-dimethylethylbenzene, or
4-ethyl-2-methyltoluene

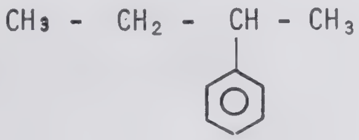


5-ethyl-3-methyl-1-propylbenzene,
5-ethyl-3-methylpropylbenzene, or
3-ethyl-5-propyltoluene

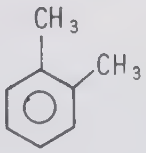
Nomenclature of Aromatic Hydrocarbons

1. Name the following aromatic hydrocarbons. (More than one name may be acceptable.)

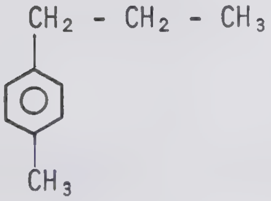
a.



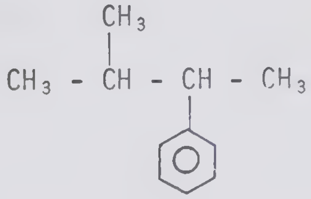
b.



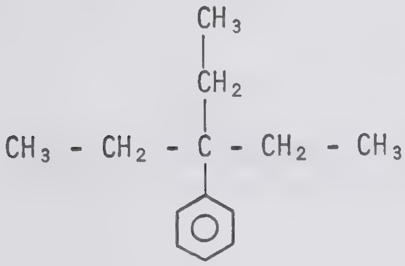
c.



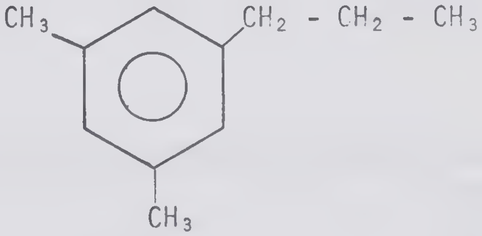
d.



e.



f.



2. Draw structural formulas for the following compounds.

a. butylbenzene

b. 3-phenylhexane

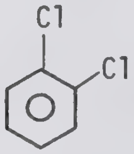
c. *o*-ethylpropylbenzene

d. 1-methyl-3-propylbenzene

e. 3-ethyl-3-phenylpentane

f. 2, 2-dimethylphenylhexane
(2, 2-dimethyl-1-phenylhexane)

3. The structural formula for 1, 2-dichlorobenzene (also called *o*-dichlorobenzene) is



Draw structural formulas for two additional isomers of this compound and give their names.

Shape of Benzene

In the benzene ring each carbon atom has three bonds and zero lone pairs therefore the shape around each carbon is trigonal planar. When the six carbons are linked together a planar hexagonal structure results.

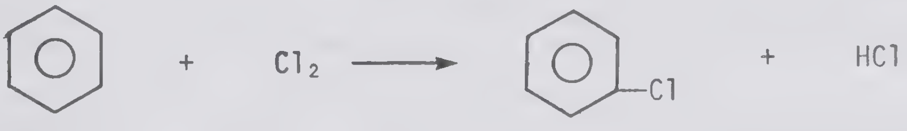
ORGANIC CHEMISTRY
AROMATICS

Physical Properties of Benzene

Benzene is a liquid at room temperature, boiling at 80.1°C. Like the aliphatics, benzene is nonpolar and hence insoluble in water.

Chemical Properties of Benzene

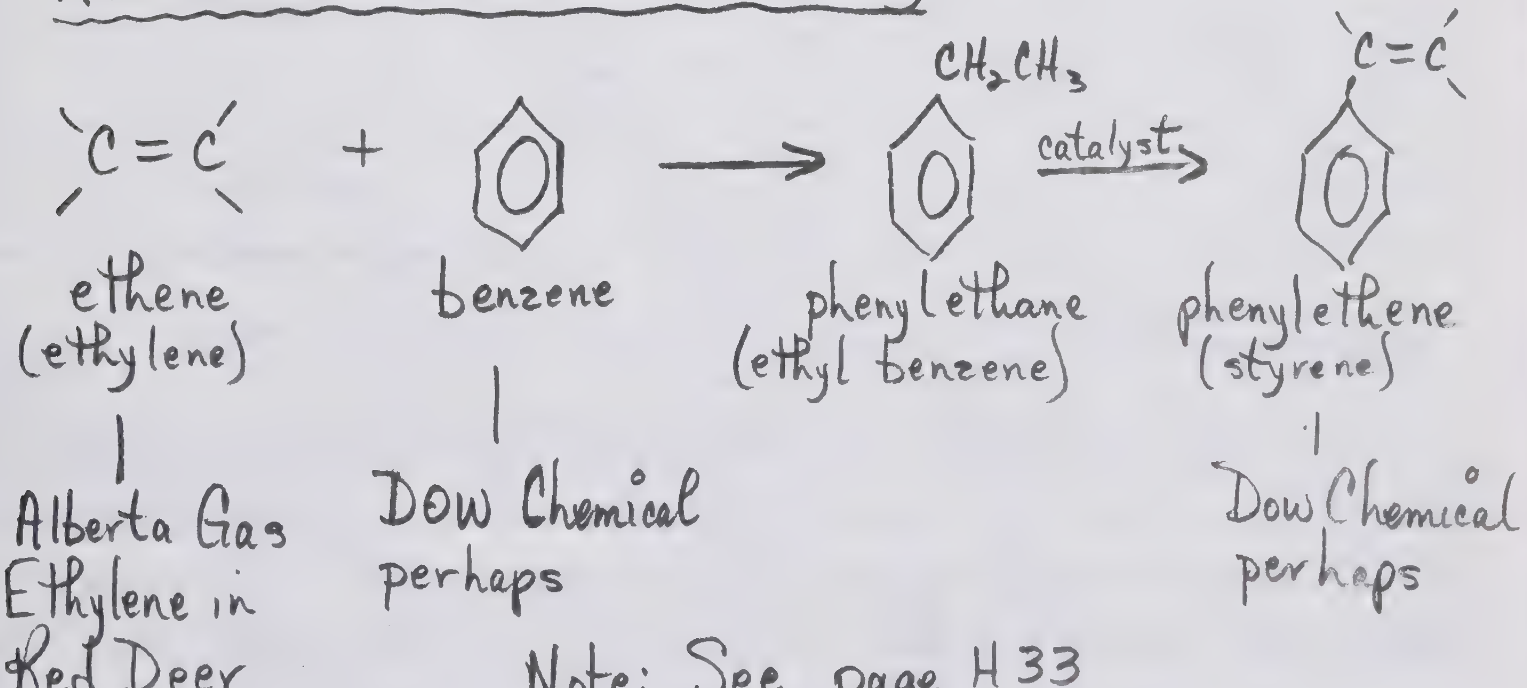
The cyclic structure of benzene is unusually stable and remains intact in most of its chemical reactions. The benzene ring reacts like an alkane. It does not take part in addition reactions but rather undergoes substitution. For example, the reaction between benzene and chlorine is



Some Sources and Uses of Aromatics

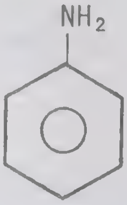
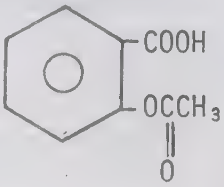
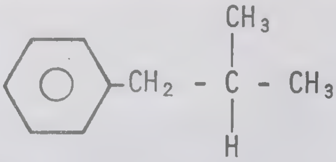
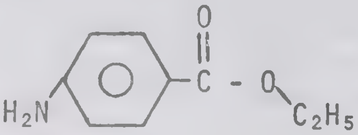
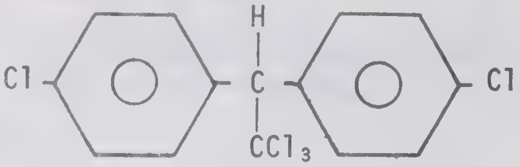
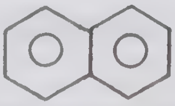
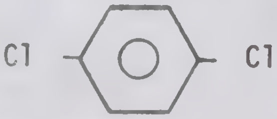
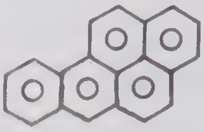
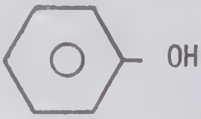
The principal source of aromatic compounds is coal tar. Coal tar is a black gummy material obtained when soft coal is destructively distilled (heated in the absence of air). Fractional distillation and chemical processing of coal tar yields a large variety of aromatic compounds which serve as starting materials for the synthesis of a multide of products including low-lead gasoline, dyes, plastics, pesticides, explosives, preservatives, and drugs and medicines. Some examples of the many aromatic compounds are given in Table H3.

Alberta's Petrochemical Industry

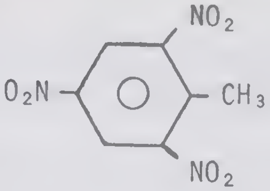
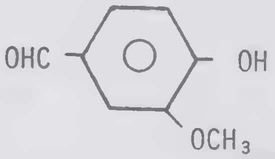
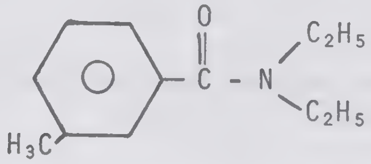


Note: See page H 33

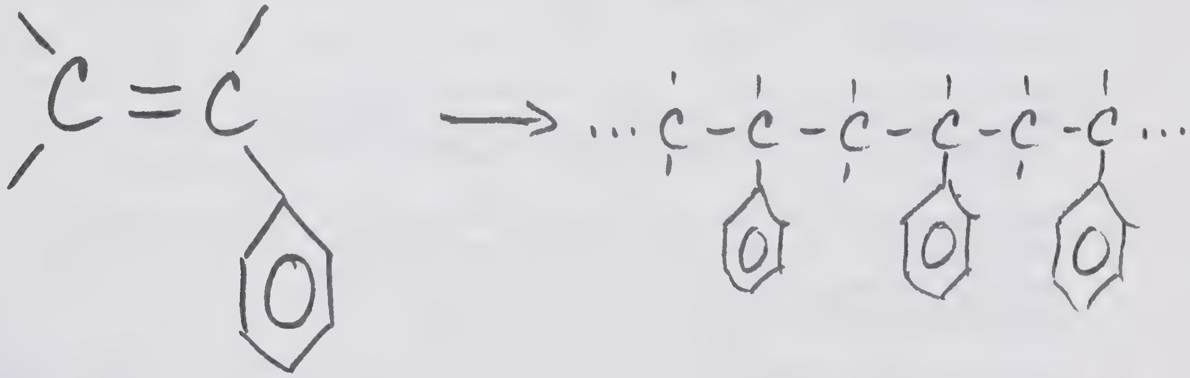
Table H3
Some Common Aromatics

Name	Structure	Uses(s)
aniline		production of: dyes, perfumes, varnishes, medicines
aspirin (acetylsalicylic acid)		relief of pain
benzedrine		central nervous system stimulant; decongestant
benzocaine		local anesthetic
D. D. T.		insecticide
naphthalene		moth killer
1, 4-dichlorobenzene (paradichlorobenzene)		moth repellant
benzopyrene		carcinogen (a compound that may induce cancer) present in cigarette smoke
phenol		germicides, disinfectants

SOME COMMON AROMATICS

trinitrotoluene (TNT)		explosive
vanillin		the compound that is responsible for the vanilla flavor
N, N-diethyl-m-toluamide		insect repellant

Alberta's Petrochemical Industry



phenylethene (styrene) – a monomer used in the production of polystyrene

Note:

Dow Chemical in Fort Saskatchewan did have plans for a benzene-styrene plant. However, because of Dow's involvement in a new vinyl chloride monomer plant and the expansion of their ethylene oxide – ethylene glycol and ethylene chloride plants, the benzene-styrene plant has been set aside for now.

REACTIONS OF CYCLOHEXANE, CYCLOHEXENE AND BENZENE - LAB H2

Purpose:

To investigate the effect of structure of hydrocarbons (saturation and unsaturation) upon their relative reactivity and upon the kind of reactions they undergo (substitution or addition).

Materials:

3 - 13 x 100 mm test tubes
1 - test tube rack
3 - stoppers or corks for test tubes
1 - reagent bottle of cyclohexane
1 - reagent bottle of cyclohexene
1 - reagent bottle of benzene
1 - reagent bottle of Br_2 - CCl_4 solution
1 - reagent bottle of $KMnO_4$ solution
3 - medicine droppers (if reagents are not provided in dropping bottles)
1 - wash bottle containing distilled water
- blue litmus paper

Part A: Reaction of Br_2 with Cyclohexane, Cyclohexene and Benzene

Procedure:

1. Into three separate labelled test tubes add 1 mℓ (20 drops) of cyclohexane, cyclohexene and benzene.

2. Add 5 - 6 drops of Br_2 - CCl_4 solution to each of the three hydrocarbons. Lightly stopper and shake the contents of each. (NOTE: CCl_4 takes no active part in the reaction and serves only as the solvent for Br_2.)

3. Note and record in the data table the name of the hydrocarbon(s) which immediately decolorize(s) the bromine. (The disappearance of the characteristic reddish-brown color of bromine upon addition to a hydrocarbon indicates the bromine has reacted with the hydrocarbon.)

4. Successively unstopper then lower a moist piece of blue litmus paper close to the level of the hydrocarbon in each of the test tubes. Note and record in the data table any changes that occur. (The only product of the reactions involved in their experiment which will render blue litmus pink is HBr gas whose aqueous solution is acidic. The evolution of HBr gas suggests a substitution reaction in which one Br atom from Br_2 replaces a hydrogen atom of a hydrocarbon molecule. The substituted hydrogen atom then combines with the second Br atom from Br_2 to form HBr gas.)

5. Place stoppers lightly into the test tubes containing the reaction mixture and place them under a U. V. lamp or some other strong light source. After ten minutes repeat the litmus test described in Step 4. Record the observations in the data table.

REACTIONS OF CYCLOHEXANE, CYCLOHEXENE AND BENZENE - LAB H2

Data:

Hydrocarbon	Color Change Immediately After Adding Br_2	Effect Upon Litmus Paper Initially	Color Change After Ten Minutes	Effect Upon Litmus Paper After Ten Minutes
Cyclohexane				
Cyclohexene				
Benzene				

Part B: Reactions of $KMnO_4$ with Cyclohexane, Cyclohexene and Benzene

Procedure:

1. Into three separate labelled test tubes add about 1 mℓ (20 drops) of cyclohexane, cyclohexene and benzene.
2. Add 2 mℓ of the potassium permanganate, $KMnO_4$, solution to each of the three test tubes containing the hydrocarbons.
3. Place a stopper lightly in each test tube and shake each gently.
4. After about one minute note and record, in the data table, any changes in color appearing in the test tubes. (The disappearance of the characteristic purple color of the permanganate solution indicates a chemical reaction has occurred.)
5. Shake the test tubes every two minutes and record the color change again after about 5 minutes.

Hydrocarbon	Color Change After One Minute	Color Change After Five Minutes
Cyclohexane		
Cyclohexene		
Benzene		

REACTIONS OF CYCLOHEXANE, CYCLOHEXENE AND BENZENE - LAB H2

Questions:

Part A:

1. Of the hydrocarbons considered,
   a. which reacts most readily with Br_2?

   b. which slowly reacts with Br_2?

   c. which appears not to react with Br_2?

2. Which of the hydrocarbons react with bromine by
   a. substitution?

   b. addition?

3. Compare saturated and unsaturated aliphatics with respect to
   a. their reactivity and

   b. the kind of reaction they tend to undergo (substitution or addition).

REACTIONS OF CYCLOHEXANE, CYCLOHEXENE AND BENZENE - LAB H2

Part B:

4. a. What can be concluded about the relative reactivity of cyclohexane, cyclohexene and benzene?

   b. How do the results relating to reactivity observed in Part A compare with those observed in Part B?

5. (optional). If one of the hydrocarbons appeared not to react either with Br_2 and $KMnO_4$ in this experiment, does this necessarily indicate that the particular hydrocarbon will not react with these reagents under other conditions?

Description of Hydrocarbon Derivatives

Numerous organic compounds are considered derivatives of hydrocarbons; i. e., derived from hydrocarbons, in the sense that a *functional group* appears in the compound in place of one or more hydrogen atoms. Functional groups usually contain elements other than carbon and hydrogen. The most common other element is oxygen and comparatively less common are nitrogen, the halogens and sulfur.

When hydrocarbon derivatives undergo reactions, only a small portion, the functional group, is usually changed. Therefore, by remembering the behaviour of one functional group in a reaction, the products of many reactions can be predicted. For example, a mixture of ethanol and hydrogen bromide reacts to give water and ethyl bromide.

$$CH_3 - CH_2 - \underset{\substack{\text{functional}\\ \text{group}}}{\textcircled{OH}} + HBr \longrightarrow CH_3 - CH_2 - \underset{\substack{\text{new functional}\\ \text{group}}}{\textcircled{Br}} + H_2O$$

In the above reaction only the functional groups changed. The alkyl part of each molecule remains the same. From this reaction and the functional group concept, the following general equation can be written.

$$R - OH + HBr \longrightarrow R - Br + H_2O$$

The hydrocarbon derivatives that will be considered include organic halides, alcohols, carboxylic acids and esters.

Bonding in Organic Halides

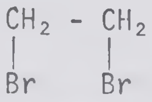
When one or more hydrogen atoms of a hydrocarbon are replaced with halogen atoms, the resulting compound is called an organic halide. The functional group in an organic halide is a monoatomic halogen.

Nomenclature of Organic Halides

Organic halides are named by adding the prefix *fluoro*, *chloro*, *bromo* or *iodo* to the name of the parent hydrocarbon. The number of added halide atoms is indicated by an appropriate prefix. Note the following examples.

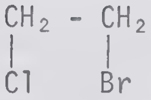
CH_3Cl

monochloromethane



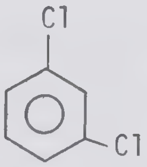
$\underset{Br}{\underset{|}{CH_2}} - \underset{Br}{\underset{|}{CH_2}}$

1, 2-dibromoethane



$\underset{Cl}{\underset{|}{CH_2}} - \underset{Br}{\underset{|}{CH_2}}$

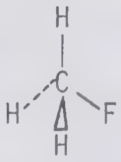
1-chloro-2-bromoethane



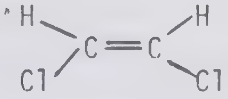
1, 3-dichlorobenzene, or
o-dichlorobenzene

Shapes of Organic Halides

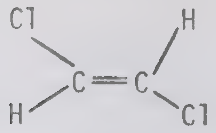
Halogens tend generally to form only a single bond. The shape around the carbon to which one or more halides are bonded may be assumed to be roughly similar to that of the corresponding hydrocarbon. However, it should be remembered that the presence of the halide would tend to somewhat modify the symmetry of the molecule. More importantly, the presence of halide atoms in the molecule would likely cause it to become polar. The polarity would depend upon the symmetry of the molecule and upon the number of bonded halide atoms. The following examples should serve to illustrate these ideas.



modified tetrahedral shape; molecule is polar



modified trigonal planar shape around each carbon; molecule is polar



modified trigonal planar shape
around each carbon; molecule
is nonpolar

Physical Properties of Organic Halides

The common organic halides are liquids under ordinary conditions. However, those that are methane derivatives, such as trichloromethane, $CHCl_3$ are quite volatile. Among the organic halides, the iodides have the highest boiling points, followed by the bromides, chlorides and fluorides in that order. This is explainable in terms of van der Waals forces associated with the respective halogen atoms.

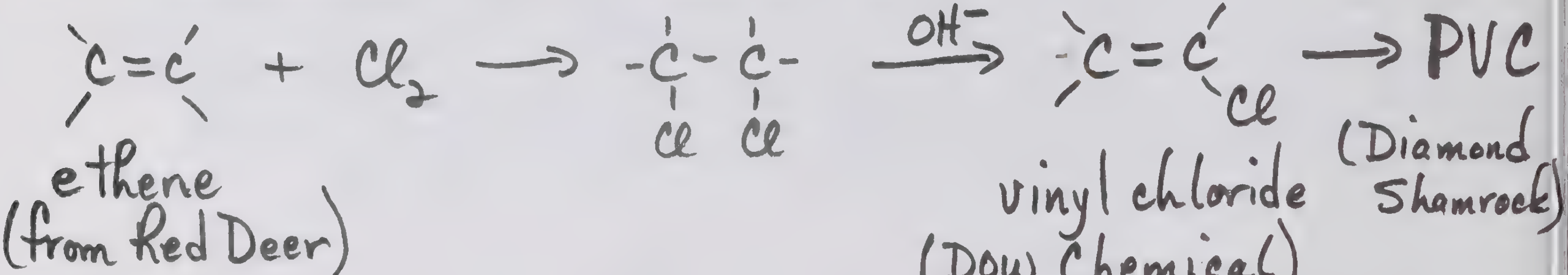
The organic halides are generally insoluble in water, but soluble in other nonpolar solvents. Even the polar organic halides have low solubility in water because of their only-slight polarity.

Chemical Properties of Organic Halides

A particularly important use of organic halides is in the synthesis of a large variety of organic compounds. The versatility of the halides in such synthesis is due to the ease with which the halogen atom is replaced by other functional groups. An example of such a replacement is given below.

$$OH^- + CH_3CH_2Cl \longrightarrow CH_3CH_2OH + Cl^-$$

Alberta's Petrochemical Industry



Note: Government approval has been given for an ethene plant in Red Deer and vinyl chloride and polyvinyl chloride (PVC) plants in Fort Saskatchewan.

ORGANIC CHEMISTRY

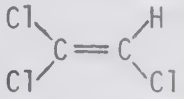
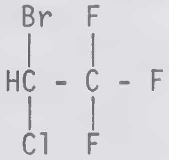
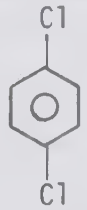
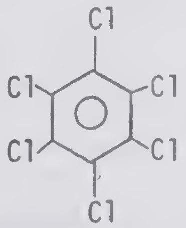
ORGANIC HALIDES

Some Organic Halides and Their Uses

H8

Table H4
Organic Halides and Their Uses

H41

Name (Common Name in Brackets)	Structural Formula	Typical Uses
trichloromethane (chloroform)	$CHCl_3$	good solvent, general anaesthetic, sedative, antiseptic
triiodomethane (iodoform)	CHI_3	antiseptic
tetrachloromethane (carbon tetrachloride)	CCl_4	good solvent
dichlorodifluoromethane (freon)	CF_2Cl_2	refrigerant fluid; propellant for non food aerosol products
1, 1, 2-trichloroethene		dry-cleaning solvent
2-bromo-2-chloro-1, 1, 1-trifluoroethane	 $\underset{Cl}{\overset{Br}{HC}} - \underset{F}{\overset{F}{C}} - F$	general inhalation anaesthetic
1, 4-dichlorobenzene or *p*-dichlorobenzene		component of common moth repellant
hexachlorocyclohexane (lindane)		agricultural insecticide

Bonding in Alcohols

Alcohols are compounds that have an OH or hydroxyl functional group bonded to a carbon atom or alkyl chain. Their general formula can be represented as ROH, where R is an alkyl group. Unlike inorganic hydroxides (NaOH, KOH), alcohols are nonionic and do not produce OH^- ions in aqueous solution. Generally, only single bonds are present in simple alcohols; thus most alcohols are saturated compounds. All bonds in an alcohol are covalent, but the O - H bond is polar and the shorter chain alcohols involve hydrogen bonding among its molecules.

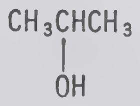
Nomenclature of Alcohols

The IUPAC names of alcohols containing one *OH* group is obtained by dropping the final *e* and adding the suffix *ol* to the name of the particular hydrocarbon. The position of the *OH* group on the alkyl chain is indicated by the number of the carbon atom to which it is attached.

Compounds containing more than one *OH* group are also classed as alcohols. The use of the suffixes *diol* and *triol* is used for their IUPAC names. Study the examples given below.

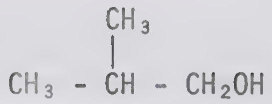
$CH_3CH_2CH_2OH$

1-propanol



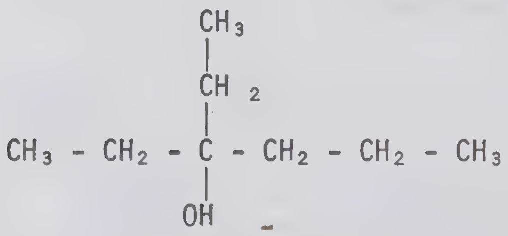
$$\begin{array}{c} CH_3CHCH_3 \\ | \\ OH \end{array}$$

2-propanol



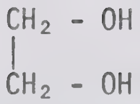
$$\begin{array}{ccccc} & & CH_3 & & \\ & & | & & \\ CH_3 & - & CH & - & CH_2OH \end{array}$$

2-methyl-1-propanol



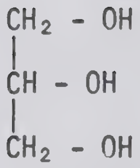
$$\begin{array}{ccccccccccc} & & & & CH_3 & & & & & & \\ & & & & | & & & & & & \\ & & & & CH_2 & & & & & & \\ & & & & | & & & & & & \\ CH_3 & - & CH_2 & - & C & - & CH_2 & - & CH_2 & - & CH_3 \\ & & & & | & & & & & & \\ & & & & OH & & & & & & \end{array}$$

2-ethyl-2-hexanol



$$\begin{array}{l} CH_2 - OH \\ | \\ CH_2 - OH \end{array}$$

1, 2-ethanediol
(ethylene glycol)



$$\begin{array}{l} CH_2 - OH \\ | \\ CH - OH \\ | \\ CH_2 - OH \end{array}$$

1, 2, 3-propanetriol
(glycerin)

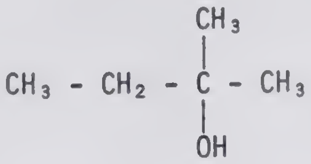
ORGANIC CHEMISTRY
ALCOHOLS

Nomenclature of Alcohols

1. Give the name for each of the following alcohols.

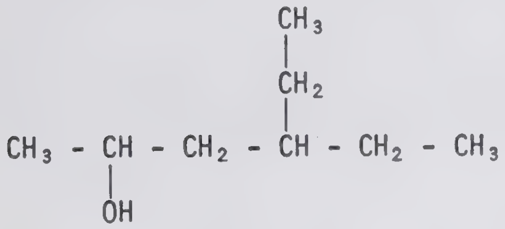
a. $CH_3 - CH_2 - CH_2 - CH_2OH$

b.



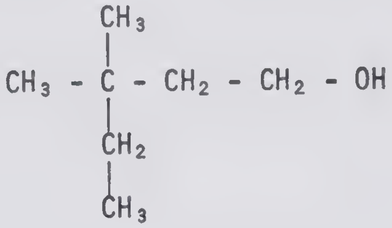
$CH_3 - CH_2 - C(CH_3)(OH) - CH_3$

c.



$CH_3 - CH(OH) - CH_2 - CH(CH_2CH_3) - CH_2 - CH_3$

d.



$CH_3 - C(CH_3)(CH_2CH_3) - CH_2 - CH_2 - OH$

2. Give the structural formulas for the following alcohols.

a. 2-butanol

b. 1-pentanol

c. 4-propyl-3-heptanol

d. 1, 3-propanediol

e. 2, 2-dimethylpropanol

f. 1-phenyl-2-butanol

3. Give the structural formulas and names for 6 isomers of pentanol.

Shape Associated with the OH Group in Alcohols

The Lewis diagram for an alcohol group is

$$R\ \ :\ddot{\underset{\cdot\cdot}{O}}:\ \ H$$

Surrounding the oxygen atom are two bonds and two lone electron pairs. Thus, the orientation around the oxygen atom is V-shaped.

Physical Properties of Alcohols

The physical properties of alcohols significantly differ from those of hydrocarbons or organic halides. This difference is due primarily to hydrogen bonding among alcohol molecules. As a result, the melting and boiling points of alcohols are much higher than the melting and boiling points of the corresponding alkanes or organic halides. For example, the boiling point of methanol is 64.5°C, that for methane is -161°C and that for monochloromethane is -23.7°C.

Because alcohols involve hydrogen bonds, they are more soluble in water than the corresponding hydrocarbons or organic halides. The lower alcohols are completely miscible with water. In these compounds the hydroxyl group comprises an appreciable portion of the molecule. Attraction between the water and alcohol dipoles is significant. As the number of carbon atoms in the alcohol molecule increases, the water solubility decreases because the alcohol is becoming more like a hydrocarbon and less like water. For example, 1-hexanol is only slightly soluble in water but highly soluble in hexane.

Chemical Properties of Alcohols

Alcohols exhibit wide versatility in their ability to react with other species. As a result the reactions of alcohols are extensive and varied. For present purposes, the discussion is being limited to two kinds of reactions--combustion and esterification.

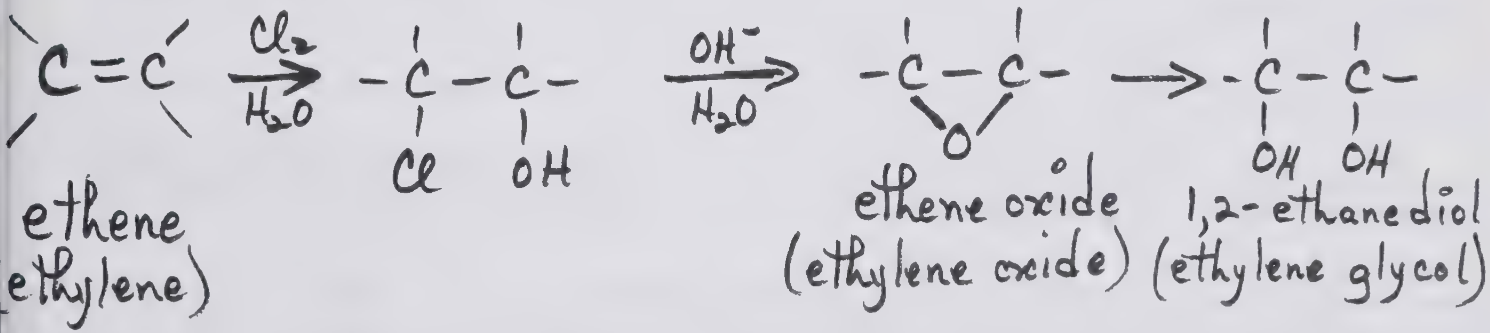
Alcohols, like most hydrocarbons, readily burn. (Alcohol lamps were common before being replaced by electricity because alcohols burn with a clean bright flame.) The following reaction illustrates the burning (combustion) of alcohols.

$$2CH_3OH + 3O_2 \longrightarrow 2CO_2 + 4H_2O$$

Ethanol, present in alcoholic beverages, is *burned* in the body by what is usually called *oxidation*. The reaction rate for oxidation is slow compared to combusion.

Esterification reactions will be discussed in the section on organic acids.

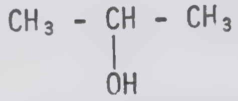
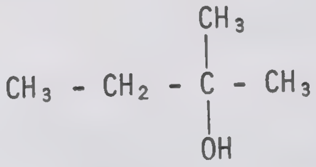
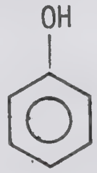
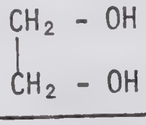
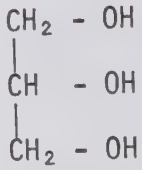
Alberta's Petrochemical Industry



Dow Chemical at Fort Saskatchewan has cheap supply f chlorine and sodium hydroxide from its chlor-alkali electrolysis of aqueous sodium chloride) plant. With an abundant supply of ethene from Red Deer, Dow will expand its existing ethylene oxide-ethylene glycol plant.

Uses of Some Common Alcohols

TABLE H5
Common Alcohols

Names (Common Name in Brackets)	Structural Formula	Typical Uses
methanol (methyl alcohol, or wood alcohol)	CH_3OH	gas line and windshield washer antifreeze; solvent for varnishes and shellacs; denaturant for ethanol
ethanol (ethyl alcohol, or grain alcohol)	CH_3CH_2OH	alcoholic beverages; in pharmaceutical industry as solvent and medicinal ingredient; in industry as solvent and antifreeze
2-propanol	 $CH_3 - \underset{\displaystyle OH}{\underset{\mid}{CH}} - CH_3$	rubbing alcohol; solvent
1-butanol	$CH_3 - CH_2 - CH_2 - CH_2 - OH$	solvent; hydraulic fluid
2-methyl-2-butanol	 $CH_3 - CH_2 - \overset{\displaystyle CH_3}{\overset{\mid}{\underset{\displaystyle OH}{\underset{\mid}{C}}}} - CH_3$	solvent; medicines; flotation agent
phenol (carbolic acid)		germicide; component of some plastics. Reactions different from those of nonaromatic alcohols
1, 2-ethanediol (ethylene glycol)	 $\begin{array}{l} CH_2 - OH \\ \mid \\ CH_2 - OH \end{array}$	radiator antifreeze
1, 2, 3-propanetriol (glycerin)	 $\begin{array}{l} CH_2 - OH \\ \mid \\ CH - OH \\ \mid \\ CH_2 - OH \end{array}$	cosmetics; pharmaceuticals; inks; candy; raw material for some explosives

ORGANIC CHEMISTRY
ALCOHOLS

Methanol

Methanol (methyl alcohol, methyl hydrate or wood alcohol) is the simplest alcohol. The principal source of this alcohol used to be the destructive distillation of wood, hence the name wood alcohol. Methanol is highly toxic, causing blindness and death. Methanol is used often as a media for organic reactions, as a solvent for varnishes and shellacs, as a gas line antifreeze, duplicating fluid and for denaturing ethanol.

Ethanol

Ethanol (ethyl alcohol or grain alcohol) is the second member of the alcohol series. It is probably most familiar because it is the essential ingredient in alcoholic beverages. Ethanol has relatively low toxicity. However its long-term, excessive use is known to cause various undesirable effects such as cirrhosis of the liver. The ethanol that is designated for beverage use is carefully controlled and heavily taxed. Any ethanol that is used industrially is generally tax free but is denatured to prevent its use as a beverage. *Denaturing* is done by the addition of some agent that is disagreeable and probably poisonous.

Ethanol destined for beverage use is produced by yeast fermentation of liquids containing simple sugars or other carbohydrates, such as starch or cellulose. A reaction involved in the fermentation of glucose is

$$\underset{\text{glucose}}{C_6H_{12}O_6} \xrightarrow{\text{yeast}} 2C_2H_5OH + 2CO_2$$

Ethanol destined for industrial uses is generally prepared by hydrating ethene. This method involves the following reaction.

$$CH_2 = CH_2 + H_2O \xrightarrow[H_2SO_4]{} CH_3CH_2OH$$

The product from this reaction yields the fairly pure ethanol (96% ethanol and 4% water) that is required for reagent purposes. For some applications the ethanol can be further purified to 100% (absolute alcohol).

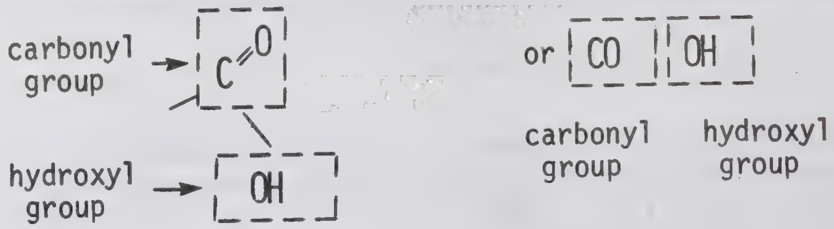
Alcoholic beverages produced by fermentation consists of two types--undistilled and distilled. The main undistilled beverages are beer, wine and champagne. The distilled beverages include whiskey, gin, rum and brandy. Undistilled beverages have a much lower alcohol content than the distilled.

Beer is produced by the fermentation of malted (germinated) grain. It usually contains from 3 to 5% alcohol. Hops, the dried cones of a special vine is added to beer to give it a bitter taste.

Wine and champagne are produced by the fermentation of grape juice. The natural wines produced by the fermentation process alone usually have an alcoholic content no higher than 15%. (Fermentation stops when the ethanol concentration reaches that level.) An alcoholic content of 15% corresponds to a proof value of 30, the proof being double the alcoholic percentage by volume. Some wines (fortified wines) contain added alcohol and may have an alcoholic content as high as 20%. Champagne wine is bottled so that it retains dissolved carbon dioxide, although some cheaper champagnes are artificially carbonated.

Bonding of Carboxylic Acids

Organic acids, known as carboxylic acids, are characterized by the functional group called a *carboxyl* group. The carboxyl group (COOH) consists of a *carbonyl* group with a *hydroxyl* group attached to the carbon atom.

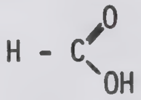
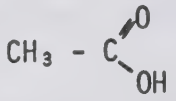
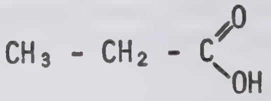
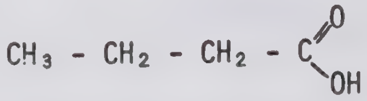
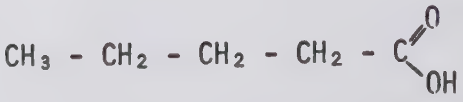


The carboxyl group is covalently bonded to hydrogen in the simplest acid and to a hydrocarbon chain for most of the other organic acids.

Nomenclature of Carboxylic Acids

Carboxylic acids are named in the IUPAC system by dropping the *e* and adding the suffix *oic* to the name of the parent hydrocarbon (containing the *same total number* of carbon atoms). The resulting name is then followed by the word acid. Many carboxylic acids are naturally occurring and have common or trivial names that reflect their natural source. The IUPAC and common names are given in the examples in Table H6. Additional names are given in Table H7 in the section *Sources and Uses of Some Common Organic Acids*.

Table H6
Some Simple Carboxylic Acids

Formula	IUPAC Name	Common Name
 $H - C\begin{smallmatrix} \diagup\!\!\diagup O \\ \diagdown OH \end{smallmatrix}$	methanoic acid	formic acid
 $CH_3 - C\begin{smallmatrix} \diagup\!\!\diagup O \\ \diagdown OH \end{smallmatrix}$	ethanoic acid	acetic acid
 $CH_3 - CH_2 - C\begin{smallmatrix} \diagup\!\!\diagup O \\ \diagdown OH \end{smallmatrix}$	propanoic acid	propionic acid
 $CH_3 - CH_2 - CH_2 - C\begin{smallmatrix} \diagup\!\!\diagup O \\ \diagdown OH \end{smallmatrix}$	butanoic acid	butyric acid
 $CH_3 - CH_2 - CH_2 - CH_2 - C\begin{smallmatrix} \diagup\!\!\diagup O \\ \diagdown OH \end{smallmatrix}$	pentanoic acid	valeric acid

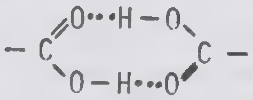
ORGANIC CHEMISTRY
CARBOXYLIC ACIDS

Shape of Carboxylic Acids

The shape around the carbon atom in the carboxyl group can be determined by noting that the carbon atom has three bonds and no lone electron pairs. This gives a trigonal planer shape to the carboxyl functional group.

Physical Properties of Carboxylic Acids

Carboxylic acids have higher melting and boiling points than hydrocarbon, organic halides or alcohols with the same number of carbon atoms. The acids containing one to ten carbon atoms are liquids at room temperature, the higher nembers are waxlike solids. The higher melting and boiling points of the organic acids are due mainly to strong hydrogen bonding. Carboxylic acids have even higher melting and boiling points than alcohols because of the special nature of the hydrogen bonding. In organic acids, there is hydrogen bonding to the oxygen of the carbonyl group as well as the oxygen of the ydroxyl group.



Organic acids containing one to four carbon atoms are completely miscible with ater. Those acids having six or more carbon atoms are almost insoluble in water. This eflects the interactions between the polar and nonpolar parts of the molecule in etermining the properties of substances. The short-chain molecules have small nonpolar ortions and are soluble in water. The long-chain molecules have large nonpolar portions nd have very low solubility in water but good solubility in nonpolar solvents.

hemical Properties of Organic Acids

Organic acids have properties like that of inorganic acids, except, in general, hey are weaker acids. Like inorganic acids, they similarly affect indicators, react ith active metals and carbonates, and are neutralized by bases. In addition, they react ith alcohols, in a reaction comparable to neutralization, to form compounds called sters. The esterification reaction involved will be discussed in the section dealing ith esters.

ources and Uses of Some Common Carboxylic Acids

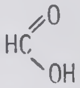
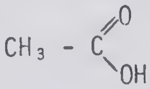
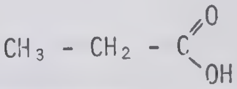
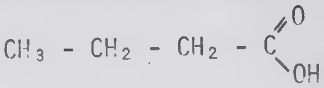
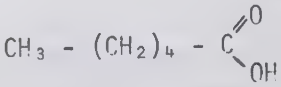
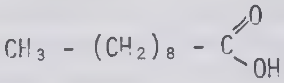
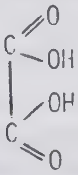
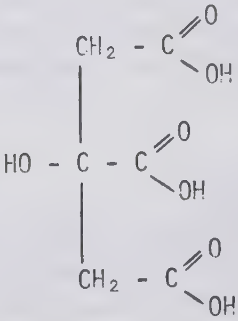
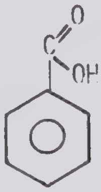
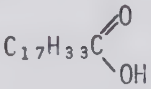
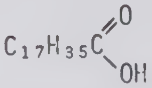
Many carboxylic acids are present in various fruits and imparts to them the sour aste characteristic of acids. An important source of longer chain organic acids are imal fats and vegetable oils. Table H7 following gives the source and use of some mmon organic acids.

ORGANIC CHEMISTRY

CARBOXYLIC ACIDS

Table H7

Sources and Uses of Some Carboxylic Acids

Name (Common Name in Brackets)	Formula	Sources and Typical Uses
methanoic acid (formic acid)		stinging agent of red ants, used in medicine and food preservatives, used in manufacture of formica
ethanoic acid (acetic acid)		ingredient in vinegar, used as a solvent and in photography
propanoic acid (propionic acid)		salts used as mold inhibitor in baking industry; used as an emulsifier
butanoic acid (butyric acid)		odor-causing agent in rancid butter; flavoring agent
hexanoic acid (caproic acid)		characteristic odor of limburger cheese, used as a flavoring agent
decanoic acid (capric acid)		characteristic odor of goats
ethanedioic acid (oxalic acid)		poisonous material present in leaves of such plants as rhubarb; used as a cleaning agent
2-hydroxy-1, 2, 3-propanetrioic acid (citric acid)		present in citrus fruits; used as flavoring agent in foods
benzoic acid		acid or salts used as a food preservative
oleic acid		found in vegetable oils
stearic acid		found in beef tallow
cerotic acid	$C_{25}H_{51}COOH$	found in beeswax, sheep tallow

ORGANIC CHEMISTRY
ESTERIFICATION - LAB H3

Purpose:

To prepare some common esters and to note their characteristic odor.

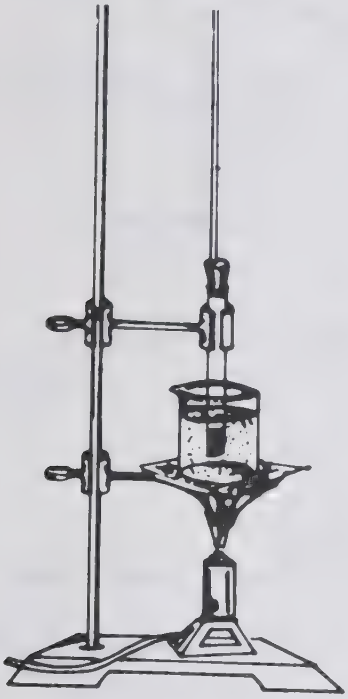


Figure K2

Materials:

- 4 - 18 x 150 mm test tubes
- 1 - #1 one-hole rubber stopper
- 1 - 50 cm length of 6 mm glass tubing
- 1 - dropper bottle of concentrated H_2SO_4
- 1 - dropper bottle of methanol
- 1 - dropper bottle of ethanol
- 1 - dropper bottle of 1-butanol
- 1 - dropper bottle of 2-butanol
- 1 - dropper bottle of 1-pentanol
- 1 - dropper bottle of 2-pentanol
- 1 - dropper bottle of glacial ethanoic acid (glacial acetic acid)
- 1 - dropper bottle of pentanoic acid
- 1 - bottle of salicylic acid
- 1 - 250 mℓ beaker
- 1 - utility clamp
- 1 - ring stand
- 1 - ring
- 1 - wire gauze
- 1 - bunsen burner

Procedure:

1. Set up a 250 mℓ beaker on a ring stand using a ring and a wire gauze. Fill the beaker with water to about the two-thirds level. This is to serve as a water bath. See Figure K2.

2. Use a utility clamp to support a 18 x 150 mm test tube. Lower the test tube into the water bath. See Figure K2.

3. Check the odor of salicylic acid and methanol.

   Precaution: Use your hand to waft the odor towards your nose. Do not smell directly.

4. Place about 2 mℓ of salicylic acid into the supported test tube (to a depth of about 1 cm or fingernail width).

5. Add about 2 mℓ of methanol to the salicylic acid in the test tube (to an additional depth of about 1 cm or 1 fingernail width).

6. Add about 10 drops of concentrated sulfuric acid to the mixture in the test tube.

7. Insert the stopper and glass tubing into the test tube. See Figure K2.

   (The glass tubing serves as a reflux condenser which condenses volatile components and returns them into the test tube.)

8. Heat the water bath until the reaction mixture starts to bubble slowly. Continue moderate heating for about 5 minutes.

9. Allow the reaction mixture to cool for several minutes. Remove the condenser and check the odor of the ester formed in the test tube (odor of wintergreen).

10. Repeat procedure Steps 1 through 9 for each of the following combinations of an organic acid with an alcohol.

    a. glacial ethanoic acid and ethanol (sweet fruit odor; used in some brands of nail polish remover)

    b. glacial ethanoic acid and 1-butanol (odor of raspberries)
    (Optional: If 2-butanol is used, then an ester with odor of strawberries is produced.)

    c. glacial ethanoic acid and 1-pentanol (odor of pears)
    (Optional: If 2-pentanol or 3-pentanol is used, then an ester with the odor of bananas is produced.)

    d. pentanoic acid and 1-pentanol (odor of apples).

QUESTIONS:

1. What specific evidence indicates that a chemical reaction has occurred in each case?

2. (Optional) Write a structural equation to represent each of the esterification reactions that were done. Name the compounds reacted and produced.

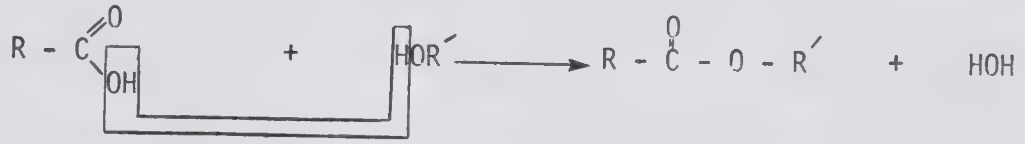
ORGANIC CHEMISTRY
ESTERS

Esters

Esters are best studied by considering the esterification reaction first.

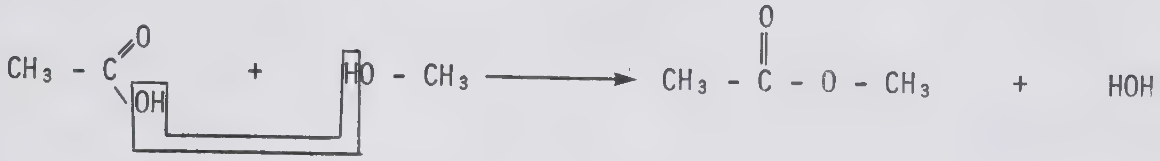
Esterification Reaction

carboxylic acid + alcohol ⟶ ester + water



$$R - C\overset{\displaystyle O}{\underset{\displaystyle OH}{}} + HOR' \longrightarrow R - \overset{O}{C} - O - R' + HOH$$

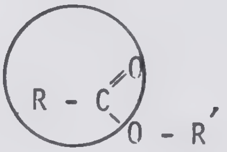
Example:



$$CH_3 - C\overset{\displaystyle O}{\underset{\displaystyle OH}{}} + HO - CH_3 \longrightarrow CH_3 - \overset{O}{\overset{\|}{C}} - O - CH_3 + HOH$$

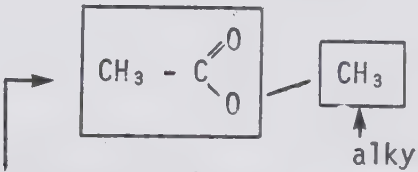
Nomenclature of Esters

A general formula for esters is



$$R - C\overset{\displaystyle O}{\underset{\displaystyle O - R'}{}}$$

where the circled part is derived from the acid and the - O - R is the alkyl part derived from the alcohol. In the naming of an ester, the alkyl (alcohol) name is given first, followed by the name of the acid part. In the IUPAC system, when naming the acid part, drop the ending *-ic* and replace it with *-ate*. Consider the following examples.

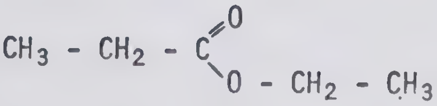


$$CH_3 - C\overset{\displaystyle O}{\underset{\displaystyle O}{}} - CH_3$$

For naming purposes, the part considered derived from the organic acid, named ethanoate (or acetate)

alkyl part of alcohol, named methyl

Full name of ester—methyl ethanoate (or methyl acetate)



$$CH_3 - CH_2 - C\overset{\displaystyle O}{\underset{\displaystyle O - CH_2 - CH_3}{}}$$

ethyl propanoate
(or ethyl propionate)

$CH_3 - CH_2 - COO - CH_2 - CH_3 - CH_3$

propyl propanoate
(or propyl propionate)

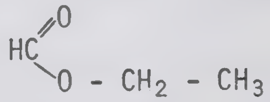
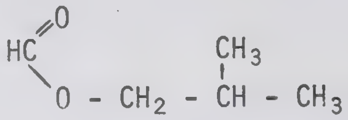
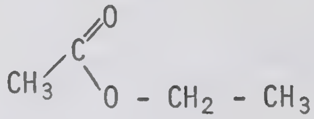
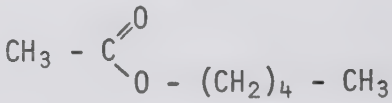
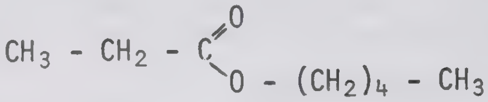
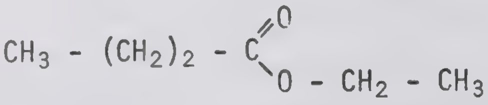
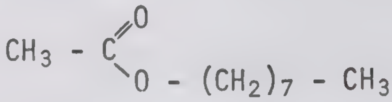
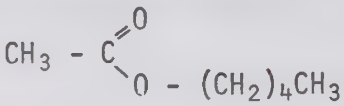
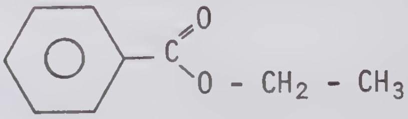
$CH_3 - CH_2 - CH_2 - COO - CH_2 - CH_2 - CH_3$

propyl butanoate
(or propyl butyrate)

Sources and Uses of Some Common Esters

Esters are a common occurrence in nature and are abundant in animal fats and vegetable oils. Unlike the acids involved in their formation, simple esters usually have pleasant odors and constitute the odors and flavors of fruits. Table H8 gives some examples of esters.

Table H8
Sources and Uses of Some Common Esters

Name (Common Name is Given in Brackets)	Formula	Sources and Typical Uses
ethyl methanoate (ethyl formate)		rum flavor and odor
2- methylethyl methanoate (isobutyl formate)		raspberry flavor and odor
ethyl ethanoate (ethyl acetate)		fingernail polish remover, solvent
pentyl ethanoate (n-amyl acetate)		banana flavor and odor
pentyl propanoate (pentyl propionate)		apricot flavor and odor
ethyl butanoate (ethyl butrate)		used in artificial peach, pineapple and apricot flavors
octyl ethanoate (octyl acetate)		orange flavor and odor
pentyl ethanoate (isoamyl acetate)		pear flavor and odor
ethyl benzoate		cherry flavor and odor

Esters and Esterification

1. Write a structural equation to represent a reaction between each of the following. Name the products in each case.

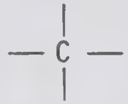
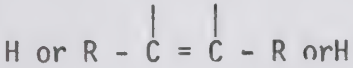
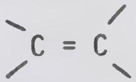
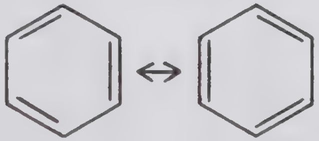
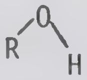
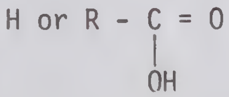
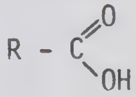
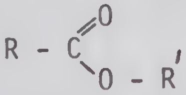
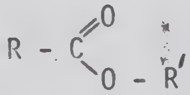
   a. butanol and propanoic acid

   b. hexanoic acid and pentanol

   c. penatanoic acid and hexanol

   d. hexanoic acid and pentanol

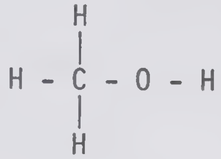
ORGANIC CHEMISTRY
SUMMARY TABLE FOR SOME ORGANIC COMPOUNDS

GROUP	STRUCTURE (R REPRESENTS CARBON CHAIN)	NOMENCLATURE	SHAPE	a) PHYSICAL PROPERTIES b) CHEMICAL REACTIONS	USES AND OCCURRENCE
alkanes	—	— ane	 $-\overset{\vert}{\underset{\vert}{C}}-$ tetrahedral around each C atom	a) non polar; insoluble; low melting and boiling points b) substitution; combustion	fuels
alkenes	 $H \text{ or } R-\overset{\vert}{C}=\overset{\vert}{C}-R \text{ or} H$	— ene	 trigonal planar around each C atom	a) same as alkanes b) addition	starting materials for many plastics
alkynes	$H \text{ or } R-C \equiv C-R \text{ or} H$	— yne	$-C \equiv C-$ linear around each C atom	a) same as alkanes b) addition of one or two molecules of adding reagent	first member of the series used in oxyacetylene welding
aromatics		variable	each C atom in the ring has a trigonal planar shape around it. Molecule is a planar hexagon	a) non polar; insoluble in water b) substitution; no addition	very diverse--solvents, foods, drugs, explosives, mothballs
alcohols	$R-OH$	— anol	 V-shaped around the O atom	a) higher boiling; soluble because of hydrogen bonding b) many reactions, e. g., esterification, combustion	very diverse--antifreeze, alcoholic drinks, cosmetics, foods
acids	 $H \text{ or } R-\underset{\underset{OH}{\vert}}{C}=O$	— anoic acid	 trigonal planar around C	a) high boiling; soluble due to hydrogen bonding b) all inorganic acid reactions; esterification	commonly occur in foods, waxes
esters		— yl — anoate	 trigonal planar around C	a) insoluble in water b) can react with water to form an acid and alcohol	used as solvents and artificial flavors; commonly occur in animal fats and vegetable oils

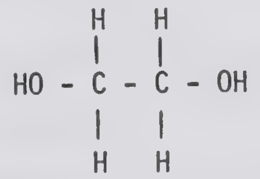
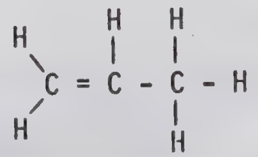
ORGANIC CHEMISTRY REVIEW
ORGANIC NOMENCLATURE AND USES OF SOME ORGANIC COMPOUNDS

H2-10

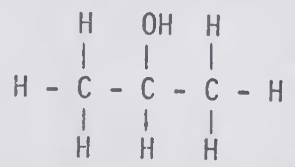
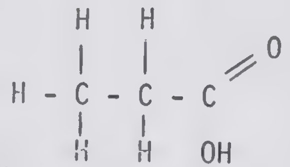
Fill in the following table.

	NAME	MOLECULAR FORMULA	STRUCTURAL FORMULA	USE
1.				heating homes
2.			 $H-\overset{\overset{H}{\vert}}{\underset{\underset{H}{\vert}}{C}}-O-H$	
3.	methylbenzene (toluene)			solvent for many glues
4.		C_2H_4		
5.	ethanoic acid			
6.				dynamite (TNT or trinitrotoluene)

ORGANIC CHEMISTRY REVIEW

	NAME	MOLECULAR FORMULA	STRUCTURAL FORMULA	USE
7.		C_2H_2		
8.			 $HO-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-OH$	
9.		C_6H_5OH		Lysol disinfectant
10.		$C_3H_5(OH)_3$		
11.				a lighter fluid
12.	propane			
3.			 ${}^{H}_{H}\!>C=\overset{H}{C}-\underset{H}{\overset{H}{C}}-H$	

ORGANIC CHEMISTRY REVIEW

	NAME	MOLECULAR FORMULA	STRUCTURAL FORMULA	USE
14.	ethanol			
15.	*p*-dichlorobenzene			
16.			 $H-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{OH}{C}}-\underset{H}{\overset{H}{C}}-H$	
17.	butanoic acid			
18.			 $H-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{OH}{C}=O$	
19.		CF_2Cl_2		
20.		$CHCl_3$		

RGANIC CHEMISTRY REVIEW

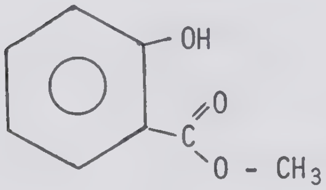
Review of Organic Chemistry

1. If "R" represents an alkyl group, name the class of organic compounds that the following general formulas can represent.

General Formula	Class of Organic Compounds
R - H	
R - X (where X ≡ halogen)	
R - OH	
R - COOH	
R - COO - R′	

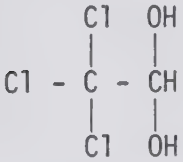
2. Identify the group or groups present in each of the following compounds.

a. Methyl salicylate or oil of wintergreen (a pain killer and a flavoring agent):



hydroxyl, ______________________

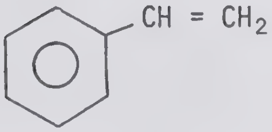
b. chloral hydrate (a sedative)



$\mathrm{Cl-C(Cl)_2-CH(OH)_2}$

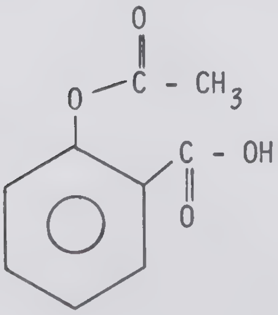
____

c. styrene (plastics monomer)



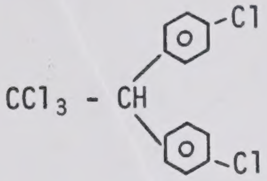
____

d. acetyl-α-salicyclic acid (aspirin)



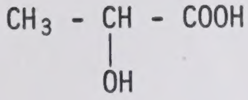
____

e. dichlorodiphenyl trichloroethane (DDT)



____

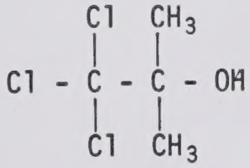
f. 2-hydroxypropanoic acid (lactic acid found in sour milk)



$$CH_3 - \underset{\displaystyle OH}{\underset{|}{CH}} - COOH$$

____

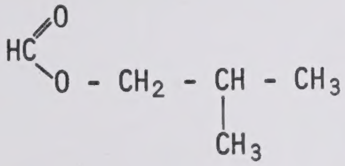
g. 3, 3,' 3-trichloro-2-methyl-2-propanol (a sedative)



$$Cl - \underset{\underset{\displaystyle Cl}{|}}{\overset{\overset{\displaystyle Cl}{|}}{C}} - \underset{\underset{\displaystyle CH_3}{|}}{\overset{\overset{\displaystyle CH_3}{|}}{C}} - OH$$

____

h. 2-methyl propylmethanoate (partially responsible for odor of raspberries)



$$HC(=O)-O - CH_2 - \underset{\displaystyle CH_3}{\underset{|}{CH}} - CH_3$$

____

3. Account for the variation in boiling point among the following two-carbon molecules.

Compound	Boiling Point (°C)
ethane	-88.6
monochloroethane	12.2
ethanol	78.5
propanoic acid	141.1

DATE DUE SLIP

EDUC FE 7 '79
DUE Educ FEB 12 '79
FEB 12 RETURN
DUE EDUC MAR 14 '83
RETURN MAR 14 '83
DUE EDUC JAN 26 '85
JAN 29 RETURN
EDUC MAR 15 '85
EDUC MAR 21 '85
MAR 21 RETURN
DUE EDUC MAR 22 '90
MAR 19 RETURN
DUE EDUC MAR 14 '91
MAR 01 RETURN
DUE EDUC. OCT 16 '92

1992 OCT 13 RETURN
RETURN FEB -1 '97

F255

JUL 7 1977

QD 41 A3312 1976 UNIT H C-3
ALBERTA CHEMISTRY PROJECT
MATERIALS
ALCHEM 20
39283345 CURR
000020715900

RECOMMENDED FOR USE
IN ALBERTA SCHOOLS

QD 41 A3312 1976 Unit H C. 3
Alberta Chemistry Project
Materials.
ALCHEM 20.
0187415B CURR

c. 3

CURRICULUM
EDUCATION LIBRARY

B15943